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(19) World Intellectual Property Organization International Bureau





(43) International Publication Date 13 February 2003 (13.02.2003)

(10) International Publication Number WO 03/012089 A2

(51) International Patent Classification7:

C12N 9/00

(21) International Application Number: PCT/GB02/03461

(22) International Filing Date:

26 July 2002 (26.07.2002)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

60/308,366

26 July 2001 (26.07.2001) US

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- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW.

(84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Declarations under Rule 4.17:

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- as to applicant's entitlement to apply for and be granted a patent (Rule 4.17(ii)) for the following designations AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG)
- of inventorship (Rule 4.17(iv)) for US only

Published:

without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: NOVEL BACE PROTEINS, NUCLEIC ACID MOLECULES THEREFOR, NOVEL CRYSTAL STRUCTURE OF NOVEL BACE PROTEINS, AND METHODS FOR MAKING AND USING

(57) Abstract: Disclosed and claimed are novel BACE proteins, crystal structures thereof, nucleic acid molecules therefor, and methods for making and using and uses of the same, especially for ascertaining inhibitors of BACE; and thus, disclosed and claimed too are inhibitors of BACE and methods of making and using the same.



5 TITLE OF THE INVENTION

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NOVEL BACE PROTEINS, NUCLEIC ACID MOLECULES THEREFOR, NOVEL CRYSTAL STRUCTURE OF NOVEL BACE PROTEINS, AND METHODS FOR MAKING AND USING FIELD OF THE INVENTION

This invention relates generally to structural studies of the soluble Beta-site APP cleaving enzyme (BACE) catalytic domain (e.g., the aspartyl protease domains of BACE) and the corresponding structural information obtained by X-ray crystallography.

Moreover, the present invention relates to any one or more of:

A catalytic domain of BACE, or a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or apo-BACE crystals which are BACE crystals with no ligand bound, regardless of the source of the BACE) and/or apo-BACE crystals which are capable of being soaked with ligand to give complexes and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a=236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02\AA or $105.02\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $105.02\text{\AA} \pm \text{cell variability of } 3\text{\AA}$, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing;

Apo-BACE crystals that can be soaked, e.g., with ligands such as inhibitory or modulatory ligands, to give complexes, such as protein-ligand complexes;

A crystalline form of BACE or a BACE that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site or apo-BACE crystals with no ligand bound, regardless of the source of the BACE; for instance, for use in rational drug design, as well as methods for ligand screening and design by X-ray crystallography;

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BACE proteins comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure (included in the term "BACE proteins") - such as those, when compared with other BACE proteins (such as Genbank accession P56817) have one or more of: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453) - whereby such proteins can also optionally include one or more of: a tag such as a His tag (e.g., a HIS6 tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from

BACE proteins that have one or more mutations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals, such as with reference to Genbank accession P56817: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453);

incomplete pro-peptide cleavage (and separation if required);

BACE proteins that include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of

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the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required);

One or more nucleic acid molecules (e.g., an isolated nucleic acid molecule) encoding the BACE proteins or at least a functional portion thereof including any of the foregoing proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure including those having reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the foregoing;

Vectors or cells (e.g., viral vectors such as baculovirus, bacterial vectors such as *E. coli*, mammalian cells such as CHO cells, or DNA plasmids) containing and/or expressing any one or more of the nucleic acid molecules and/or BACE proteins – the latter can include prior BACE proteins especially when there is co-expression thereof with a gene product - an enhancer - that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, for instance a convertase or a transcription enhancer or a translation enhancer or both a transcription and translation enhancer, for instance a prohormone convertase such as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells, and thus also vectors or cells containing and/or expressing the nucleic acid molecules and/or BACE proteins and a nucleic acid molecule encoding the enhancer as well as kits containing separately packaged isolated nucleic acid molecules comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer, for use in vectors or cells for the co-expression thereof;

Expression through or by vectors or cells of that which is encoded by the nucleic acid molecules and/or contained in the aforementioned vectors or cells and/or of the gene products and/or the amino acid sequences and/or the BACE proteins, including co-expression thereof, or of other nucleic acid molecules encoding BACE proteins, with a gene product that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, e.g., a convertase, for instance a prohormone convertase such

WO 03/012089

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as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells;

Methods for crystallizing BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain;

Methods for determining the crystal structure of BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain;

Uses of that which is encoded by the nucleic acid molecules and/or the gene products and/or the amino acid sequences and/or the BACE proteins, for instance in screening assays such as drug or patient screening assays or in generating products therefor (such as for generating antibodies to the catalytic domain and/or to BACE proteins which are useful in such assays), as well as such assays and products therefor, and uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells, for preparing such uses or assays and/or components for such uses or assays;

Products from such assays ("assay products"), as well as uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells for preparing such assay products and/or components for such assay products;

Inhibitors or modulators of BACE and/or inhibitors or modulators of the production of A β or fragments thereof, for instance, such inhibitors or modulators as determined through the assays of the present invention and/or through contact with and binding to or otherwise inhibiting or modulating BACE proteins of the present invention, such as a compound or composition which binds to and/or inhibits and/or modulates and/or interacts with a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2Å) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of

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BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing (excluding, of course, prior known inhibitors, modulators, if any, of BACE and/or inhibitors, modulators of the production of A β or fragments thereof);

Uses of such assay products and/or inhibitors and/or modulators, for instance in treating maladies, conditions, diseases and the like such as Alzheimer's disease (AD) involving BACE activity and/or Aβ or fragments thereof and/or in formulating medicaments for such treatments, as well as of uses of the nucleic acid molecules, vectors or cells, the methods and/or the aforementioned expression via vectors or cells, for such treatment and/or a component thereof and/or for preparing such medicaments and/or a component thereof, such that methods for preparing such medicaments including use of any of the foregoing is included, *inter alia*.

And a data storage medium encoded with the structural co-ordinates of crystallized BACE or at least a functional portion thereof. Such data storage material is capable of displaying such structures, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure co-ordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using structure co-ordinates to screen and design compounds, including inhibitory compounds, that bind to BACE or homologues thereof. The present invention also relates to compositions and crystals of BACE in complex with a BACE inhibitor. *Cf.* WO 01/37194.

Various documents are cited in this text. Citations in the text can be by way of a citation to a document in the reference list, e.g., by way of author(s) and document year citation to a document listed in the reference list, or by full citation in the text to a document that may or may not also be listed in the reference list.

There is no admission that any of the various documents cited in this text are prior art as to the present invention. Any document having as an author or inventor person or persons named as an inventor herein is a document that is not by another as to the inventive entity herein.

All documents cited in this text ("herein cited documents") and all documents cited or referenced in herein cited documents are hereby incorporated herein by reference. Likewise, teachings of herein cited documents and documents cited in herein cited documents can be employed in the practice and utilities of the present invention.

BACKGROUND OF THE INVENTION

Alzheimer's disease (AD) is estimated to afflict more than 20 million people worldwide and is believed to be the most common form of dementia (Newsday (New York), Friday, July 6, 2001, City Edition, page A24). AD is a progressive dementia characterized by amyloid plaques and intracellular neurofibrillary tangles that accumulate in the brain and are thought to be responsible for the mental decline in Alzheimer's patients.

Beta-amyloid protein $(A\beta)$ is the major constituent of the amyloid plaques, which are characteristic of AD (De Strooper and Konig, 1999).

 $A\beta$ is a 39-42 amino acid residue peptide formed by the specific cleavage of a class I transmembrane protein called the amyloid precursor protein (APP) by two proteases, β - and γ -secretase (the $A\beta$ fragment).

 β -secretase cleaves APP between residues Met671 and Asp672 (numbering corresponds to the 770 amino acid isoform of APP) to form the N-terminus of A β . A second cleavage of the peptide is associated with γ -secretase to form the C-terminus of the A β peptide. β and γ -secretases cleave the amino and carboxy terminal ends of the A β domain, respectively. A third enzyme, α -secretase, has recently been identified which cleaves APP within the A β domain between residues 16 and 17 of the A β fragment (Howlett et al., 2000).

The therapeutic potential of inhibiting and/or modulating the deposition of Aβ has motivated many groups to isolate and characterize secretase enzymes and to identify their potential inhibitors (*see*, *e.g.*, WO01/23533 A2, EP0855444A2,WO00/17369, WO00/58479, WO00/47618, WO01/00665; WO01/00663; U.S. Patent No. 6,245,884 (Hook), U.S. Patent No. 6,221,667 (Reiner et al.), U.S. Patent No. 6,211,235 (Wu et al.)). Indeed, it also has been reported in the popular press that "[d]rug makers are studying medicines called gamma-secretase inhibitors, which aim to block the cleavage process" (Newsday (New York), Friday, July 6, 2001, City Edition, page A24).

Consequently, a number of potential candidates for these enzymes have recently been reported in the literature: Several groups have identified and isolated aspartate proteases that have

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β-secretase activity (Hussain et al., 1999; Lin et. al, 2000; Yan et. al, 1999; Sinha et. al., 1999 and Vassar et. al., 1999). β-secretase is also known in the literature as Asp2 (Yan et. al, 1999), Beta site APP Cleaving Enzyme (BACE) (Vassar et. al., 1999) or memapsin-2 (Lin et al., 2000).

BACE was identified using a number of experimental approaches such as EST database analysis (Hussain et al. 1999); expression cloning (Vassar et al. 1999); identification of human homologs from public databases of predicted C. elegans proteins (Yan et al. 1999) and finally utilizing an inhibitor to purify the protein from human brain (Sinha et al. 1999). Thus, five groups employing three different experimental approaches has led to the identification of the same enzyme, making a strong case that BACE is a β-secretase. Mention is also made of the patent literature: WO91/13904, EP518955, EP732399, WO92/03542, WO92/07068, WO96/40885, EP87/1720, U.S. Patents Nos. 5,942,400 and 5,744,346, EP855444, EP1037977, WO00/17369, WO01/23533, WO0047618, WO00/58479, WO01/00663, WO01/00665, EP848062, U.S. Patents Nos. 6,025,180 and 6,162,639, EP1047788 and WO99/33963, WO99/46281, WO98/11236, U.S. Patent No. 5,942,400 and WO94/13319.

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Indeed, BACE is a membrane bound protein which is synthesized as a partially active proenzyme, and is most abundantly expressed in brain tissue. It is thought to represent the major βsecretase activity.

BACE activity may be considered to be a rate-limiting step in the production of AB. This makes BACE of special interest in the pathology of Alzheimer's disease and other maladies that involve AB, or fragments thereof (e.g., amyloid plaques and amyloid angiopathy also characterize the brains of individuals with Trisomy 21 or Down's Syndrome, Hereditary Cerebral Hemorrhage with Amyloidosis of the Dutch Type (HCHWA-D), inter alia; see also U.S. Patent No. 6,211,235), and therefore an important candidate for the development of drugs as a treatment against Alzheimer's disease and/or against such other maladies.

Furthermore, as reported in the popular press, Newsday (New York), Friday, July 6, 2001, City Edition, page A24, that day's edition of Science includes in vitro findings by investigator Thomas Sudhof of the Howard Hughes Medical Institute which suggest that gamma secretase may be implicated in another function, but that it is not known if those findings apply to humans or which genes may be involved. Nonetheless, inhibiting gamma secretase may have issues which are addressed by the present invention involving inhibiting BACE the production of AB or fragments 35 thereof.

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The likelihood of developing Alzheimer's disease increases with age, and as the aging population of the world increases, this disease may become a greater and greater problem. In addition, there is a familial link to AD and consequently any individuals possessing the double mutation of APP known as the Swedish mutation (in which the mutated APP forms a considerably improved substrate for BACE) have a much greater chance of developing AD and also of developing it at an early age (see also U.S. Patent No. 6,245,964 pertaining to transgenic rodent comprising APP-Swedish).

It would therefore be useful to inhibit and/or modulate the deposition of Aβ and portions thereof; for instance by inhibiting and/or modulating BACE proteins through inhibitors or modulators thereof ascertained from BACE proteins having a particular crystal structure or having a structure as herein set forth.

Hence, drugs that reduce or block BACE activity would reduce $A\beta$ levels and levels of fragments of $A\beta$ in the brain or elsewhere where $A\beta$ or fragments thereof deposit and thus slow the formation of amyloid plaques and the progression of AD or other maladies involving deposition of $A\beta$ or fragments thereof (Yankner, 1996; De Strooper and Konig, 1999).

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Further, reaction systems comprising Beta secretase have been asserted to be useful in screening assays, e.g., to identify inhibitors or modulators and antibodies raised against Beta-secretase have been asserted to be useful for screening and other assays; see, e.g., U.S. Patent No. 6,221,645 and other documents cited herein; and thus, the present invention is likewise useful in such assays in generating antibodies.

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There has been the production of certain active recombinant BACEs - different from those of the herein invention - using heterologous expression systems for mammalian cells (Vassar et al, 1999, Hassain et al, 1999), insect cells (Mallender et al, 2001) and bacterial cells (Lin et al 2000). While the production of these BACEs shows that no undue experimentation is needed to practice the present invention, these prior systems had deficiencies addressed by the herein invention.

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Indeed, prior to the present invention there was a need to produce a soluble recombinant BACE protein with an improved crystal structure that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å ± standard

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deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2), as well as amino acid sequences therefor, nucleic acid molecules encoding them, and other aspects of the present invention as herein discussed.

In addition, the study of crystal structure and symmetry is developed (*See, e.g.*, Cotton and Wilkinson, Inorganic Chemistry (John Wiley & Sons, Fourth Ed. 1980), especially Ch. 2). X-ray crystallography, or more generally crystallography, is an established, well-studied technique that provides what can best be described as a three-dimensional picture of what a molecule looks like in a crystal, and is useful for determining whether a compound that is not a known ligand of a target biomolecule can indeed bind as a ligand to a target biomolecule (*see, e.g.*, WO 99/45379; U.S. Patent No. 6,087,478; U.S. Patent No. 6,110,672); and, there are additional techniques for identifying drug cores (*see, e.g.*, WO 98/57155 regarding fragment-based screening). Mention is also made of U.S. Patents Nos. 6,128,582, 6,153,579, 6,077,682, and 6,037,117 and PCT publications WO01/37194 and WO00/47763 for additional information on aspects of structure-based drug design and homology modelling.

These techniques can be employed with the herein disclosed BACE crystals and proteins, especially those that are without any ligands typically found in wild-type BACE, to rationally design compounds that inhibit or modulate, e.g., bind to or interact with BACE; and, the use of these techniques, in combination with herein disclosed BACE crystals and proteins it is believed has not been heretofore taught or suggested in the art.

OBJECTS AND SUMMARY OF THE INVENTION

Without excluding inventions otherwise herein disclosed, the present invention can provide one or more of the following embodiments.

The present invention in an embodiment provides a catalytic domain of BACE, such as a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates

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the need for refolding and/or a BACE protein having an unoccupied or substantially unoccupied active site (apo-BACE crystals with no ligand bound, regardless of the source of the BACE) and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3\AA , b= 105.02\AA or 105.02\AA ± standard deviation (0.2Å) or 105.02\AA ± cell variability of 3\AA , and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å or 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or $60.4\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $60.4\text{\AA} \pm \text{cell variability of 3Å}$ and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P2₁ form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

The present invention likewise provides apo-BACE crystals that can be soaked, e.g., with ligands such as inhibitory or modulatory ligands, to give complexes, such as protein-ligand complexes.

The present invention in another embodiment provides a crystalline form of BACE or a BACE that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site or apo-BACE crystals with no ligand bound, regardless of the source of the BACE; for instance, for use in rational drug design, as well as methods for ligand screening and design by X-ray crystallography.

In regard to this, the invention further provides a method for ligand screening and/or design, e.g., by X-ray crystallography and/or nuclear magnetic resonance (NMR). The method can include exposing the apo crystals or BACE crystals with no ligand bound (i.e., with an unoccupied active site, regardless of the source of the BACE) to one or more test samples, and determining whether a ligand-BACE complex is formed, e.g., obtaining an X-ray crystal diffraction pattern to

determine whether a ligand-BACE complex is formed or using NMR to determine whether such a complex is formed. The BACE can be exposed to the test samples by either co-crystallizing the BACE in the presence of the one or more test samples or soaking the BACE in a solution of one or more test samples. Structural information from ligand-BACE complexes can be used to design ligands that bind tighter, that bind more specifically, that have better biological activity or have a better safety profile. *Cf.* WO99/45379.

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The present invention thus further provides a computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain, e.g., BACE protein as herein provided and/or such information with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system: (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally complementary to said data set; (d) optionally constructing, using computer methods, a model of a chemical structure having a portion that is structurally complementary to said data set and (e) outputting to said output device the selected chemical structures having a portion complementary to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits or modulates or interacts with BACE. Cf. U.S. Patent No. 5,835,382.

In this way, one can rationally identify and/or design inhibitors or modulators of BACE or compounds that interact with BACE. And, in this regard, mention is made that the skilled artisan can employ the products found in the wild-type BACE catalytic domain as a portion of the information to be inputted or employed in the rational design and/or identification of inhibitors or modulators of BACE or compounds that interact with BACE. Furthermore, an inhibitor of BACE can be competitive, non-competitive, uncompetitive, or irreversible; and, inhibitors of BACE are of significant technical and commercial interest.

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The present invention also provides BACE proteins comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure (included in the term "BACE proteins") - such as those, when compared with other BACE proteins (such as Genbank accession P56817) have one or more of: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at an 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453) - whereby such proteins can also optionally include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification (cf. U.S. Patent No. 6,020,143); a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence (cf. U.S. Patents Nos. 6,245,532, 5,516,657); and a tag such as a HA or FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required) (cf. U.S. Patents Nos. 6,190,874, 6,083,732).

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The present invention thus further provides BACE proteins that have one or more mutations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals, such as with reference to Genbank accession P56817: a mutation at amino acid ("aa") 153 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 172 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 223 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as asparagine to glutamine, and/or a mutation at aa 354 for instance to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals such as

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asparagine to glutamine, and one or more truncations (e.g., a BACE extending from Thr 22 to Ser 453).

Advantageously, the BACE protein has all four of the mutations and the truncation.

The present invention additionally provides BACE proteins that include one or more of: a tag such as a His tag (e.g., a HIS₆ tag) for instance to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium such as a baculovirus signal sequence for example the baculovirus gp67 signal sequence; and a tag such as a FLAG tag to allow differentiation of species arising from incomplete pro-peptide cleavage (and separation if required).

Even further still, the present invention provides one or more nucleic acid molecules (e.g., an isolated nucleic acid molecule) encoding the BACE proteins or at least a functional portion thereof including any of the foregoing proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain, advantageously amino acid sequences that crystallize to the crystalline structure or a structure that mimics the crystalline structure including those having reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the foregoing.

In yet further embodiments, the present invention provides vectors or cells (e.g., viral vectors such as baculovirus, bacterial vectors such as *E. coli*, mammalian cells such as CHO cells, or DNA plasmids) containing and/or expressing any one or more of the nucleic acid molecules and/or BACE proteins – the latter can include prior BACE proteins especially when there is co-expression thereof with a gene product - an enhancer - that enhances in the particular vector or cell system, the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme e.g., a convertase, or a transcription enhancer or a translation enhancer or both a transcription and translation enhancer (*cf.*. U.S. Patents Nos. 6,130,066, 6,004,777, 5,990,091), for instance a prohormone convertase such as the prohormone convertase furin (*cf.* Laprise et al. 1998) when the vector or cell system is baculovirus and/or insect cells, and thus also vectors or cells containing and/or expressing the nucleic acid molecules and/or BACE proteins and a nucleic acid molecule encoding the enhancer as well as kits containing separately packaged isolated nucleic acid molecules for such co-expression, e.g., a kit containing separately packaged nucleic acid molecules

comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer, for use in vectors or cells for the co-expression thereof;

The invention thus also provides expression through or by vectors or cells of that which is encoded by the nucleic acid molecules and/or contained in the aforementioned vectors or cells and/or of the gene products and/or the amino acid sequences and/or the BACE proteins, including co-expression thereof, or of other nucleic acid molecules encoding BACE proteins, with a gene product that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein such as an enzyme, e.g., a convertase, for instance a prohormone convertase such as the prohormone convertase furin especially when the vector or cell system is baculovirus and/or insect cells.

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As the invention involves a unique crystal structure of BACE, the invention provides methods for crystallizing BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain.

Similarly, the invention provides methods for determining the crystal structure of BACE proteins and/or amino acid sequences and/or gene products comprising, containing, having, consisting essentially of and/or consisting of amino acid sequences of the catalytic domain.

The invention further contemplates uses of that which is encoded by the nucleic acid molecules and/or the gene products and/or the amino acid sequences and/or the BACE proteins, for instance in screening assays such as drug or patient screening assays or in generating products therefor (such as for generating antibodies to the catalytic domain and/or to BACE proteins which are useful in such assays), as well as such assays and products therefor, and uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells, for preparing such uses or assays and/or components for such uses or assays.

Included within the ambit of the present invention are products from such assays ("assay products"), as well as uses of the nucleic acid molecules, vectors or cells, methods and/or the aforementioned expression via vectors or cells for preparing such assay products and/or components for such assay products.

The BACE protein of the present invention may be employed in screening for compounds which inhibit or modulate or activate or interact with this protein. Such compounds may be identified from cells or cell fractions, mixtures of natural products or chemical libraries.

The assay may comprise mixing the BACE polypeptide of the invention with a candidate compound in solution and measuring BACE activity in the mixture. It may also be advantageous to measure binding of the compound to the BACE polypeptide (or competition with binding of a known inhibitor) instead of an effect on enzyme activity. Alternatively, versions of the BACE protein containing the transmembrane region may be expressed in cells, and these cells (or membranes prepared from these cells) may be incubated with candidate compounds. The effect on BACE activity may then be assessed by measurement of cleavage of a suitable substrate, either added to the mixture or co-expressed in the cells.

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The protein or antibodies to the protein may also be used to identify receptors, through standard techniques. These include, but are not limited to, ligand binding or cross-linking assays in which the BACE protein is labeled and contacted with a source of the putative receptor, and biophysical techniques such as surface plasmon resonance.

The present invention even further contemplates inhibitors or modulators of BACE or compounds or compositions that interact with BACE and/or inhibitors or modulators of the production of AB or fragments thereof, for instance, such inhibitors as determined through the assays of the present invention and/or through contact with and binding to or otherwise interacting with, inhibiting or modulating BACE proteins of the present invention, such as a compound or composition or ligand which binds to and/or inhibits and/or interacts with and/or modulates a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or having an unoccupied or substantially unoccupied active site and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) or 236.63Å \pm cell variability of 3\AA , b= 105.02\AA or 105.02\AA ± standard deviation (0.2Å) or 105.02Å ± cell variability of 3\AA , and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° ± standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm cell variability of 3Å, b= $107.4\text{\AA} \pm \text{standard deviation}$ (0.2Å) or $107.4\text{\AA} \pm \text{cell variability of } 3\text{\AA}$ and $c = 60.4\text{\AA}$ or $60.4\text{\AA} \pm 60.4\text{\AA}$ standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2)

and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing (excluding, of course, prior known inhibitors and modulators of BACE and/or inhibitors or modulators of the production of $A\beta$ or fragments thereof).

And, the present invention provides uses of such assay products and/or inhibitors and/or modulators and/or ligands, and/or compositions or compounds that interact with BACE, for instance in treating maladies, conditions, diseases and the like such as Alzheimer's disease (AD) involving BACE activity and/or $A\beta$ or fragments thereof and/or in formulating medicaments for such treatments, as well as of uses of the nucleic acid molecules, vectors or cells, the methods and/or the aforementioned expression via vectors or cells, for such treatment and/or a component thereof and/or for preparing such medicaments and/or a component thereof, such that methods for preparing such medicaments including use of any of the foregoing is included.

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In a further embodiment, the present invention provides a Beta-site APP cleaving enzyme which comprises an amino acid sequence of SEQ ID NO: 5; advantageously, the amino acid sequence comprises a catalytic domain, and wherein the enzyme is in a crystalline form, such as herein defined.

In another embodiment the recombinant Beta-site APP cleaving enzyme comprises an amino acid sequence of SEQ ID NO: 5 (Figs. 1B, 2A, 8), as well as nucleic acid molecules encoding such an enzyme; for instance, a nucleic acid molecule comprising a sequence of SEQ ID NO: 4 or 10 (Figs. 1A, 2B, 7).

More in particular, with respect to the herein mentioned nucleic acid molecules and polypeptides therefrom, e.g., the aforementioned nucleic acid molecules (Figs. 2B, 7) and polypeptides expressed from them (Figs. 2A, 8), the invention further comprehends isolated and/or purified nucleic acid molecules and isolated and/or purified polypeptides having at least about 70%, preferably at least about 75% or about 77% identity or homology ("substantially homologous or identical"), advantageously at least about 80% or about 83%, such as at least about 85% or about 87% homology or identity ("significantly homologous or identical"), for instance at least about 90% or about 93% identity or homology ("highly homologous or identical"), more advantageously at least about 95%, e.g., at least about 97%, about 98%, about 99% or even about 100% identity or homology ("very highly homologous or identical"; or from about 84-100% identity considered "highly conserved"); and advantageously these polypeptides obtain crystal structures as herein disclosed and the nucleic acid molecules encode polypeptides that obtain crystal structures

as herein disclosed. Moreover, it is advantageous that polypeptides of the invention have greater than 98.8% identity to herein disclosed sequences, and that nucleic acid molecules of the invention have greater than 95.6% identity to herein disclosed sequences, especially as certain amino acid sequences of the invention have 98.8% identity to sequence 32 of WO01/23533 and certain nucleic acid molecules of the invention have 95.6% identity to sequence 25 of WO01/23533 (and it is intended to exclude any prior sequences). The invention also comprehends that these nucleic acid molecules and polypeptides can be used in the same fashion as the herein or aforementioned nucleic acid molecules and polypeptides.

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Nucleotide sequence homology can be determined using the "Align" program of Myers and Miller, ("Optimal Alignments in Linear Space", CABIOS 4, 11-17, 1988, incorporated herein by reference) and available at NCBI. Alternatively or additionally, the term "homology" or "identity", for instance, with respect to a nucleotide or amino acid sequence, can indicate a quantitative measure of homology between two sequences. The percent sequence homology can be calculated as $(N_{ref} - N_{dif})^*100/N_{ref}$, wherein N_{dif} is the total number of non-identical residues in the two sequences when aligned and wherein N_{ref} is the number of residues in one of the sequences. Hence, the DNA sequence AGTCAGTC will have a sequence similarity of 75% with the sequence AATCAATC $(N_{ref} = 8; N_{dif} = 2)$.

Alternatively or additionally, "homology" or "identity" with respect to sequences can refer to the number of positions with identical nucleotides or amino acids divided by the number of nucleotides or amino acids in the shorter of the two sequences wherein alignment of the two sequences can be determined in accordance with the Wilbur and Lipman algorithm (Wilbur and Lipman, 1983, PNAS, USA 80:726, incorporated herein by reference), for instance, using a window size of 20 nucleotides, a word length of 4 nucleotides, and a gap penalty of 4, and computer-assisted analysis and interpretation of the sequence data including alignment can be conveniently performed using commercially available programs (e.g., Intelligenetics TM Suite, Intelligenetics Inc. CA). When RNA sequences are said to be similar, or have a degree of sequence identity or homology with DNA sequences, thymidine (T) in the DNA sequence is considered equal to uracil (U) in the RNA sequence (see also alignment used in Figures).

RNA sequences within the scope of the invention can be derived from DNA sequences, by thymidine (T) in the DNA sequence being considered equal to uracil (U) in RNA sequences.

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Additionally or alternatively, amino acid sequence similarity or identity or homology can be determined using the BlastP program (Altschul et al., Nucl. Acids Res. 25, 3389-3402 (1997), incorporated herein by reference) and available at NCBI. The following references (each incorporated herein by reference) provide algorithms for comparing the relative identity or homology of amino acid residues of two proteins, and additionally or alternatively with respect to the foregoing, the teachings in these references can be used for determining percent homology or identity: Needleman SB and Wunsch CD, "A general method applicable to the search for similarities in the amino acid sequences of two proteins," J. Mol. Biol. 48:444-453 (1970); Smith TF and Waterman MS, "Comparison of Bio-sequences," Advances in Applied Mathematics 2:482-489 (1981); Smith TF, Waterman MS and Sadler JR, "Statistical characterization of nucleic acid sequence functional domains," Nucleic Acids Res., 11:2205-2220 (1983); Feng DF and Dolittle RF, "Progressive sequence alignment as a prerequisite to correct phylogenetic trees," J. of Molec. Evol., 25:351-360 (1987); Higgins DG and Sharp PM, "Fast and sensitive multiple sequence alignment on a microcomputer," CABIOS, 5: 151-153 (1989); Thompson JD, Higgins DG and Gibson TJ, "ClusterW: improving the sensitivity of progressive multiple sequence alignment through sequence weighing, positions-specific gap penalties and weight matrix choice, Nucleic Acid Res., 22:4673-480 (1994); and, Devereux J, Haeberlie P and Smithies O, "A comprehensive set of sequence analysis program for the VAX," Nucl. Acids Res., 12: 387-395 (1984).

In this fashion, by comprehending nucleic acid molecules and polypeptides having such homology to the particular sequences disclosed, it is envisioned that the invention encompasses homologues to the disclosed sequences, within the herein terms.

As to homologues of the disclosed amino acid sequences (Figs 2A, 8), it is advantageous that these homologues have the herein defined crystal structure; and, as to homologues of the disclosed nucleic acid sequences, it is advantageous that these homologues encode BACE proteins having the herein defined crystal structure.

Furthermore, as to inventive nucleic acid molecules, the invention comprehends codon equivalent nucleic acid molecules. For instance, if the invention comprehends "X" protein having amino acid sequence "A" and nucleic acid molecule "N" encoding protein X, the invention comprehends nucleic acid molecules that also encode protein X via one or more different codons than in nucleic acid molecule N.

In addition, as to inventive nucleic acid molecules, the invention comprehends nucleic acid molecules that hybridize under stringent conditions to herein disclosed nucleic acid molecules.

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As to herein disclosed amino acid sequences, the invention comprehends nucleic acid molecules encoding the herein disclosed amino acid sequences, as well as nucleic acid molecules that hybridize under stringent conditions to nucleic acid molecules encoding herein disclosed amino acid sequences, as these nucleic acid molecules that hybridize under stringent conditions to nucleic acid molecules encoding herein disclosed amino acid sequences can provide proteins having similarity, homology or identity as herein discussed, especially if the proteins have the same or substantially the same crystal structure as herein disclosed.

The present invention further provides in particular embodiments a crystalline structure of both the soluble BACE catalytic domain in the presence of OM99-2 and in the absence of OM99-2, both having a space group of C2 and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P21 form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand The cell dimensions of the crystals grown in the presence of OM99-2 (Figure 3A) are a= 236.63Å, b= 105.02Å, and c= 62.59Å and β =101.32° and the asymmetric unit of the crystal containing three copies of BACE. The cell dimensions of the crystals grown in the absence of OM99-2 (Figure 3B) are a= 238.3Å, b= 107.4Å, and c= 60.4Å and β =101.89°. However, as is evident from the present disclosure, the invention is not limited by the crystals having been grown in the presence or absence of OM99-2 or anything else, and that cell dimensions can vary in all directions of the cell dimensions from a stated value, e.g., a stated cell dimension value can be that value ± standard deviation (0.2Å) or ± cell variability of 3Å, and that the stated beta angle can vary, e.g., a stated beta angle can be that value, for instance 101.32° or 101.89° or that value \pm standard deviation (0.2°) or between 101° and 108°.

BACE crystals of the present invention can have a resolution better than, i.e., numerically lower than 3Å.

The present invention further provides a method of employing the crystals of the present invention in drug screening assays, comprising selecting a potential compound which binds to the active site of the BACE catalytic domain of BACE, as well as to uses of such a compound, as herein mentioned.

The present invention further provides a data storage medium encoded with the structural co-ordinates of crystallized BACE or at least a functional portion thereof. Such data storage material is capable of displaying such structures, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure co-ordinates to solve the structure of similar or homologous proteins or protein complexes. In addition, this invention relates to methods of using structure co-ordinates to screen and design compounds, including inhibitory compounds, that bind to BACE or homologues thereof. The present invention also relates to compositions and crystals of BACE in complex with a BACE inhibitor. *Cf.* WO 01/37194.

In this disclosure, "comprises," "comprising," "containing" and "having" and the like can have the meaning ascribed to them in U.S. Patent law and can mean "includes," "including," and the like; "consisting essentially of" or "consists essentially" likewise has the meaning ascribed in U.S. Patent law and the term is open-ended, allowing for the presence of more than that which is recited so long as basic or novel characteristics of that which is recited is not changed by the presence of more than that which is recited, but excludes prior art embodiments.

These and other embodiments are disclosed or are obvious from and encompassed by, the following Detailed Description.

BRIEF DESCRIPTION OF FIGURES

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The following Detailed Description, given to describe the invention by way of example, but not intended to limit the invention to specific embodiments described, may be understood in conjunction with the accompanying Figures, incorporated herein by reference, in which:

Figure 1A shows an alignment of BACE DNA sequences (EMBL-AF190725.SEQ, EMBL-AF200343.SEQ, and EMBL-AF204943.SEQ), and a BACE DNA sequence of the present invention (BACE_dna.SEQ) (SEQ ID NOs: 1-4), illustrating the novelty, nonobviousness and inventive step of the present invention*, **;

Figure 1B shows an alignment of a BACE polypeptide sequence of the present invention (baceprot.pro) and a BACE polypeptide sequence (P56817.pro) (SEQ ID NOs: 5-6), illustrating the novelty, nonobviousness and inventive step of the present invention*, **;

Figure 2A shows an inventive BACE polypeptide sequence encoded by a BACE nucleotide sequence of the present invention (SEQ ID NO: 5);

Figure 2B shows an inventive BACE nucleotide sequence (SEQ ID NO: 4);

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Figure 3A shows a photograph from a light microscope of the BACE crystal grown in the presence of OM99-2;

Figure 3B shows a photograph from a light microscope of the BACE crystal grown in the absence of any added inhibitor (OM99-2);

Figure 4A shows a diagram providing the arrangement of BACE monomers in asymmetric unit of crystallographic cell (The blue (molecule C) and orange (molecule B) molecules of the dimer, which is homologous to the dimer of Tang et al. WO01/00663, Tang et al. WO01/00665, Hong et al., Science, 2000; 290, 150-153; the molecule in pink (molecule A) forms a dimer with a crystallographically related molecule, which is homologous to the non-crystallographic dimer);

Figure 4B shows a diagram providing the packing of the molecules in the unit cell of BACE (The pink (C), orange (B) and blue molecules (A) form the asymmetric unit, which is related to the molecules in red (D), dark blue (E) and green (F) by crystallographic symmetry);

Figure 5 shows a copy of the gel from SDS-PAGE purification of BACE;

Figure 6 shows a diagrammatic representation of the comparison between the BACE protein of the present invention versus Tang et al. WO01/00663, Tang et al. WO01/00665, Hong et al., Science, 2000; 290, 150-153 (the downward facing arrows are the sites of proteolytic cleavage; TM is the transmembrane region and cyt is the cytoplasmic region), illustrating the novelty and nonobviousness and inventive step of the present invention;

Figure 7 shows an alignment of BACE DNA sequences (e.g., Ep855444.seq, WO0100663.SEQ, and WO0123533seq25.SEQ) and a BACE DNA sequence of the present invention (BACE_dna.SEQ) (SEQ ID NOs: 7-9 and 4), illustrating the novelty and nonobviousness and inventive step of the present invention*, ***;

Figure 8 shows an alignment of BACE amino acid sequences (e.g., WO0123533SEQ32.pro and WO0100663.PRO) and a BACE amino acid sequence of the present invention (baceprot.pro) (SEQ ID NOs: 10-11, and 5), illustrating the novelty and nonobviousness and inventive step of the present invention*, ***;

- (* Figure color coded to show similarities and/or differences.)
- (** EMBL-AF190725.SEQ, EMBL-AF200343.SEQ, and EMBL-AF204943.SEQ are EMBL sequences; P56817.pro is a Genbank sequence, accession P56817.)

(*** Ep855444.seq, WO0100663.SEQ, WO0123533seq25.SEQ, WO0123533SEQ32.pro and WO0100663.PRO are sequences from European Patent Application 855444, and PCT publications WO01/00663, WO01/23533, WO01/23533 and WO01/00663.)

DETAILED DESCRIPTION

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The present invention involves a catalytic domain of BACE, or a form of BACE that is suitable for crystallization with the correct disulphide bonding. Correct disulphide bonding refers to the disulphide bonding of a biologically active conformation of a catalytic domain of BACE or a BACE protein that retains functionality. Having the correct disulphide bonding eliminates the need for refolding and/or a catalytic domain of BACE or a BACE protein having an unoccupied or substantially unoccupied active site (apo-BACE crystals with no ligand bound, regardless of the source of the BACE) and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme such as between about pH 5.6 and about pH 5.8 and/or having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å ± standard deviation (0.2Å) or 236.63Å \pm cell variability of 3Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm cell variability of 3Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm cell variability of 3Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE (e.g., from growth in the presence of OM99-2) or cell dimensions a= 238.3\AA or $238.3\text{\AA} \pm \text{standard deviation}$ (0.2Å) or 238.3Å \pm cell variability of 3Å, b= 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm cell variability of 3Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm cell variability of 3Å and β =101.89° or 101.89° \pm standard deviation (0.2°)or between 101° and 108° (e.g., from crystals grown in the absence of OM99-2) and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P21 form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

The present invention further involves the expression of these BACE proteins and their use; for instance in the rational design or identification of inhibitors or modulators of BACE.

The BACE recombinant proteins of the present invention are advantageously expressed in insect cells through a baculovirus expression system and are soluble and lack glycosylation.

Increased solubility can be achieved by C-terminal truncation of the protein to remove the transmembrane and cytoplasmic regions, while glycosylation can be removed by introducing mutations at the glycosylation sites. WO01/00663 (Tang et al.), WO01/00665 (Tang et al.), Hong et al., Science, 2000; 290, 150-153, in contrast, produced the C-terminally truncated memapsin 2 protein in bacteria for crystallization. More specifically, memapsin 2 was produced as insoluble inclusion bodies in bacteria. Therefore refolding was necessary to give a soluble, active protein. However during refolding/purification the N-terminal region was lost, due to unidentified proteolytic activity. Furthermore the final protein used for crystallization studies was a mixture of species, the majority having an N-terminus at Leu41 and a minority at Leu43 (the mature N-terminus is at Glu46). See Table 4, *infra*, for a comparison of the Tang/Hong crystal structure with the present invention.

The exemplified BACE protein was expressed with: 1) a His₆ tag added at the C-terminus to facilitate purification; 2) mutations of the asparagine residue to glutamine in the four potential glycosylation sites at amino acids 153, 172, 223 and 354, to prevent glycosylation of the protein; 3) an N-terminus generated by furin cleavage; 4) a FLAG oligopeptide tag added to the N-terminus of the pro-peptide to enable differentiation between processed and unprocessed protein and 5) a signal peptide derived from the gp67 baculoviral protein.

Possible vectors for use in the present invention, e.g., for expressing BACE or a nucleic acid molecule encoding BACE, include, but are not limited to: for insect cells, pFastBAc1 (Life Technologies), pFastBAcDual pFastBAc1 (Life Technologies), pBlueBac III or pBlueBacHis baculovirus vectors (Invitrogen, San Diego, Calif.); for bacterial cells, pET-3 (Novagen, Madison, Wis.) and for mammalian cells, pJT4 (discussed further below), pcDNA-1 (Invitrogen, San Diego, Calif.) and pSV-SPORT 1 (Gibco-BRL, Gaithersburg, Md.). Thus, any suitable vector can be used for expression of the BACE catalytic domain or proteins or for replication and/or expression of nucleic acid molecules of the invention, including e.g., in bacterial systems such as *Escherichia coli*, or in viral vector systems, and DNA plasmid systems. The methods for making a vector or recombinant or plasmid for expression of BACE or nucleic acid molecules encoding BACE can be any desired method, e.g., a method which is by or analogous to the methods disclosed herein cited documents and/or in: U.S. Patent Nos. 4,603,112, 4,769,330, 5,174,993, 5,505,941, 5,338,683, 5,494,807, 4,722,848, 4,745,051, 4,879,236, 5,762,939, 5,858,368, 6,224,882, 6,103,526, 4,769,331, 5,591,439, 5,552,143, 5,591,639, 5,589,466, 5,580,859, 6,130,066, 6,004,777,

5,990,091, and 6,156,567. However, baculovirus vector systems and insect cells are presently preferred.

The expression product generated by vectors or recombinants in this invention are advantageously isolated and/or purified from infected or transfected cells or culture medium.

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The DNA sequence coding for the BACE catalytic domain can be present in the vector operably linked to regulatory elements. In one embodiment of the present invention, insect host cells are preferably transfected with the recombinant hBACE_synth_his/pFastbac baculoviral DNA, thereby resulting in expression of the BACE catalytic domain. In another embodiment of the present invention, insect host cells are preferably transfected with the FURIN/pFastBac Dual baculoviral DNA, thereby resulting in expression of furin. Transfection and co-transfection with the recombinant molecules can be effected using methods well known in the art.

Host cells may be stably transfected or transiently transfected with a recombinant expression plasmid or infected by a recombinant virus vector. The host cells include prokaryotic cells, such as *Escherichia coli*, fungal systems such as *Saccharomyces cerevisiae*, permanent cell lines derived from insects such as *Trichoplusia ni* HighFive cells, *Spodoptera frugiperda* (SF-9) cells and *Spodoptera frugiperda* (SF-21) cells, *Spodoptera frugiperda* (SF900+, U.S. Patent No. 6,103,066), and permanent mammalian cell lines such as Chinese hamster ovary (CHO) and SV40-transformed African green monkey kidney cells (COS).

The present invention contemplates "mutants" wherein a "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native or synthetic BACE catalytic domain with a different amino acid residue and/or by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native BACE catalytic domain and which has substantially the same three-dimensional structure as the native BACE catalytic domain from which it is derived. Similarly, the present invention contemplates "mimics"; e.g., proteins that have substantially the same herein disclosed crystal structure of BACE. A mimic can be a mutant. By having substantially the same three-dimensional structure is meant having a set of atomic structure co-ordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2.0Å when superimposed with the atomic structure co-ordinates of the native BACE catalytic domain from which the mutant is derived when at least about 50% to 100% of the C_{α} atoms of the native catalytic domain are included in the superposition. A mutant or mimic may have, but need not have, β -secretase activity.

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decimal place. The co-ordinates are a relative set of positions that define a shape in three dimensions, so it is possible that an entirely different set of co-ordinates and/or space group having a different origin and/or axes and/or space group could define a similar or identical shape. Furthermore, varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e., the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5Å (preferably less than 1.0Å and more preferably less than 0.5Å) when superimposed on the co-ordinates provided in Table 5 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 5 in terms of both its structural characteristics and potency for structure-based design or identification of BACE inhibitors or modulators. Likewise, changing the number and/or positions of the water molecules and/or substrate molecules of Table 5 will not generally affect the potency of the structure for structure-based design of BACE inhibitors or modulators. Thus, for the purposes described herein as being aspects of the present invention, it is within the scope of the present invention if: the Table 5 co-ordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structures are varied so that the root mean square deviation of residue backbone atoms is less than 1.5Å (preferably less than 1.0Å and more preferably less than 0.5Å) when superimposed on the co-ordinates provided in Table 5 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the data of Table 5 accordingly includes the co-ordinate data in which one or more individual values of the Table are varied in this way. By "root mean square deviation" is meant the square root of the arithmetic mean of the squares of the deviations from the mean.

The co-ordinates of Table 5 provide a measure of atomic location in Angstroms, to a third

As used herein, "Crystal or crystalline structure" or "crystalline form": refers to a polypeptide in crystalline form. The term also includes co-crystals, as described herein. The term "co-crystal" refers to a crystal formed from a solution containing a mixture of the components i.e., polypeptide(s) and compound(s). Such compounds include, by way of example and not limitation, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc. Compounds include OM99-2, OM99-1 and a statine based peptide (Marcinkeviciene J., Luo Y., Gracian, NR., Combs Ap. And Copeland, RA. J. Biol Chem. 2001, 276:23790-23794). A soaked crystal is where a

crystal is produced from one component (polypeptide) and then the other component is soaked in the compound(s).

The "binding" which is detected between a ligand and the active site, such as to determine inhibitors of BACE is an "association" between the ligand and the active site; and "association" refers to a condition of proximity between a chemical entity or compound, or portions or fragments thereof, and the BACE catalytic domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

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The "active site" refers to that site in BACE domains where substrate peptide binding and cleavage occur. It is the site in BACE that is sought to be blocked by an inhibitor or ligand. A "functional portion" of a BACE protein includes at least the active site.

A "crystallographically-related dimer" is a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer coincide with the symmetry axes or planes of the crystal lattice, whereas a "non-crystallographically-related dimer" is a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer do not coincide with the symmetry axes or planes of the crystal lattice. And, "Bilobal structure:" refers to two globular lobes of the BACE protein and corresponds to the amino- and carboxy-terminal halves of the protein.

BACE contains a signal sequence, a pro-peptide, a catalytic aspartyl protease domain, a transmembrane region and a C-terminal cytoplasmic region. During transit through the endoplasmic reticulum, BACE undergoes constitutive N-terminal processing in the Golgi apparatus in which the pro-peptide is cleaved by a furin-like protease (Bennet et al 2000, Creemers et al 2001). More specifically, BACE undergoes a series of post-translational modifications including glycosylation, disulfide bond formation and propeptide processing. Haniu et al. have shown that BACE is N-glycosylated at four sites (Asn-153, Asn-172, Asn-223 and Asn-354) and that six Cys residues in the ectodomain form three intramolecular disulphide bonds (Cys216-Cys420, Cys278-Cys333 and Cys330-Cys380).

The present invention relates to crystalline polypeptides corresponding to the catalytic domain of BACE. Preferably, the crystalline catalytic domains are of sufficient quality to allow the determination of the three-dimensional X-ray diffraction structure to a resolution of better than, i.e., numerically lower than, 3.0Å. The invention also relates to methods for preparing and crystallizing

the polypeptides. The polypeptides themselves, as well as information derived from their crystal structures can be used to analyze and modify BACE as well as to identify compounds that interact with the catalytic domain. This can allow for the rational design or identification of compounds that inhibit or modulate BACE or interact with BACE or associate with BACE; which compounds have therapeutic value.

10 Crystalline BACE

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The crystals of the invention generally comprise substantially pure polypeptides corresponding to the BACE catalytic domain in crystalline form.

It is to be understood that the crystalline BACE catalytic domains of the invention are not limited to synthetic BACE domains. Indeed, the crystals of the invention also include native BACE catalytic domains and mutants and mimics of the BACE catalytic domain.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the BACE domain will depend, in part, on the region of the BACE domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well-known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a BACE catalytic domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the BACE catalytic domain will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit enzymatic activity. Indeed, amino acid substitutions, additions or deletions that interfere with the β -secretase activity of the BACE domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure co-ordinates obtained therefrom, can be used to identify compounds that bind to the native domain.

The co-crystals of the invention generally comprise a crystalline BACE domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

Production of Polypeptides

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The synthetic and mutated BACE catalytic domain polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Kochendoerfer GG (2001) "Chemical protein synthesis methods in drug discovery". Current Opinion in Drug Discovery and Development 4, 205-214). Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the synthetic or mutated BACE domain polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989.

A variety of host-expression vector systems may be utilized to express the synthetic BACE domain coding sequence. These include but are not limited to insect cell systems infected with recombinant virus (e.g., baculovirus) containing the BACE domain coding sequence or animal cell systems; microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the BACE domain coding sequence and yeast transformed with recombinant yeast expression vectors containing the BACE domain coding sequence. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; in bacterial systems, inducible promoters such as pL of

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bacteriophage .mu., plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used and when generating cell lines that contain multiple copies of the BACE catalytic domain DNA, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Crystallization Of Polypeptides And Characterization Of Crystal Structure

The crystals of the invention can be obtained by conventional means as are well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see, e.g., McPherson, 1982; McPherson, 1990; Webber, 1991).

Generally, the crystals of the invention are grown by dissolving substantially pure synthetic BACE domain polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

In a preferred embodiment of the invention, native crystals are grown by vapor diffusion in hanging drops (McPherson, 1982 and 1990). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, equal volumes of a substantially pure polypeptide solution are mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand, usually for about 2-6 weeks, until crystals grow.

Thus, the invention provides a method for crystallizing BACE which comprises producing a BACE protein, e.g., by recombinant production via a suitable host and/or vector such as through expression in insect cells, recovering the BACE and growing crystals from the recovered BACE. The BACE so produced is suitable for X-ray diffraction analysis. And, the growing of the crystals can be by any suitable means, advantageously the hanging drop method.

Uses of the Crystals and Atomic Structure Co-ordinates

The crystals of the invention, and particularly the atomic structure co-ordinates obtained therefrom, have a wide variety of uses. The crystals (either apo or co-complexed) and structure co-

ordinates (either apo or co-complexed) are particularly useful for identifying compounds that inhibit β -secretase activity as an approach towards developing new therapeutic agents.

The structure co-ordinates described herein can be used as phasing models in determining the crystal structures of additional synthetic or mutated BACE domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, etc. The structure co-ordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of synthetic or mutated BACE domains, such as those obtained via nuclear magnetic resonance (NMR).

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The provision of the structure of BACE crystals in Table 5 provides the skilled artisan with a detailed insight into the mechanisms of action of BACE. This insight provides a means to design inhibitors of BACE which can be used for inhibiting BACE or the production of A β or fragments thereof or treating AD or disorders involving the production of A β or fragments thereof (which disorders are treatable by inhibition of BACE) in an individual in need thereof.

The provision of the crystal structure of BACE allows a novel approach for drug discovery, identification, and design for modulators, e.g., inhibitors, of BACE. Accordingly, the invention provides a computer-based method of rational drug design or identification which comprises: providing the structure of BACE as defined by the co-ordinates or the identifying co-ordinates in Table 5; providing a structure of a candidate modulator or inhibitor; and fitting the structure of the candidate to the structure of BACE of Table 5.

In an alternative aspect, the method may use the co-ordinates of atoms of interest of BACE which are in the vicinity of the active site or binding region in order to model the pocket in which the substrate or ligand binds. These co-ordinates may be used to define a space which is then screened "in silico" against a candidate modulator molecule. Thus, the invention provides a computer-based method of rational drug design or identification which comprises: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"); providing the structure of a candidate modulator or inhibitor; and fitting the structure of the candidate to the selected co-ordinates of BACE.

In practice, it may be desirable to model a sufficient number of atoms of BACE as defined by the co-ordinates of Table 5 which represent the active site or binding region. Thus, there can be provided the co-ordinates of at least 5, advantageously at least 10, more advantageously at least 50 and even more advantageously at least 100 atoms of the BACE structure.

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Accordingly, the methods of the invention can employ a sub-domain of interest of BACE which is in the vicinity of the active site or binding region, and the invention can provide a computer-based method for identifying or rationally designing a drug which comprises: providing the co-ordinates of at least a sub-domain of BACE; providing the structure of a candidate modulator or inhibitor of BACE; and fitting the structure of the candidate to the co-ordinates of the BACE sub-domain provided.

These methods can optionally include synthesizing the candidate and can optionally further include contacting the candidate with BACE to test whether there is binding and/or inhibition.

"Fitting" can mean determining, by automatic or semi-automatic means, interactions between at least one atom of the candidate and at least one atom of BACE and calculating the extent to which such an interaction is stable. Interactions can include attraction, repulsion, brought about by charge, steric considerations, and the like. A "sub-domain" can mean at least one, e.g., one, two, three, or four, complete element(s) of secondary structure. Particular regions of BACE include those identified in Table 5.

Modulators of BACE may be inhibitors of BACE or compounds which affect its specificity or activity in other ways. Advantageously, modulators are inhibitors.

The step of providing the structure of a candidate modulator molecule may involve selecting the compound by computationally screening a database of compounds for interaction with the active site. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the active site. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor can be a type of virtual pharmacophore.

In any event, the determination of the three-dimensional structure of BACE provides a basis for the design of new and specific modulators for BACE. For example, from knowing the three-dimensional structure of BACE, computer modelling programs may be used to design or identify different molecules expected to interact with possible or confirmed active sites such as binding sites or other structural or functional features of BACE.

More specifically, a potential modulator of BACE activity can be examined through the use of computer modeling using a docking program such as GRAM, DOCK or AUTODOCK (see Walters et al. Drug Discovery Today, vol. 3, no. 4 (1998), 160-178, and Dunbrack et al. Folding

and Design 2 (1997), 27-42) to identify potential inhibitors of BACE. This procedure can include computer fitting of potential modulators to BACE to ascertain how well the shape and the chemical structure of the potential modulator (e.g., inhibitor) will bind to the enzyme.

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Also, computer-assisted, manual examination of the active site or binding site of BACE may be performed. The use of programs such as GRID (P. Goodford, J. Med. Chem, 1985, 28, 849-57) – program that determines probable interaction sites between molecules with various functional groups and the enzyme surface – may also be used to analyze the active site or binding site to predict partial structures of modulating compounds.

Computer programs can be employed to estimate the attraction, repulsion or steric hindrance of the two binding partners, e.g., BACE and a candidate inhibitor. Generally, the tighter the fit, the fewer the steric hindrances, and the greater the attractive forces, the more potent the potential modulator, since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a candidate modulator, the more likely it is that it will not interact with other proteins as well. This will tend to minimize potential side-effects due to unwanted interactions with other proteins.

In a further aspect the invention provides for a method for determining the structure of a modulator of BACE bound to BACE, said method comprising, (a) providing a crystal of BACE according to the invention, (b) soaking the crystal with said modulator; and (c) determining the structure of said BACE-modulator complex.

The invention further involves, in place of or in addition to *in silico* methods, high throughput screening of compounds to select compounds with binding activity. Those compounds which show binding activity may be selected as possible candidate modulators, and further crystallized with BACE, e.g., by co-crystallization or by soaking, for X-ray analysis. The resulting X-ray structure may be compared with that of Table 5 for a variety of purposes. For example, where the contacts made by such compounds overlap with those made by BACE, novel molecules comprising residues which contain contacts of BACE and other compounds may be provided.

Having designed, identified, or selected possible binding candidate modulators or inhibitors by determining those which have favorable fitting properties, e.g., strong attraction between a candidate and BACE, these can be then screened for activity. Consequently, the invention further involves: obtaining or synthesizing the candidate modulator or inhibitor; and contacting the candidate modulator or inhibitor with BACE to determine the ability of the candidate to inhibit or

modulate or interact with BACE. In the latter step, the candidate is advantageously contacted with BACE under conditions to determine its function. Instead of, or in addition to, performing such an assay, the invention may comprise: obtaining or synthesizing the candidate modulator, forming a complex of BACE and the candidate, and analyzing the complex, e.g., by X-ray diffraction or NMR or other means, to determine the ability of the candidate to interact with BACE. Detailed structural information can then be obtained about the binding of the candidate to BACE, and in light of this information, adjustments can be made to the structure or functionality of the potential modulator, e.g., to improve its binding to BACE. These steps may be repeated and re-repeated as necessary. Advantageously, in the contacting step, the potential modulator is contacted with BACE in the presence of a substrate and typically a buffer, to determine the ability of the potential modulator to alter the function of BACE.

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The invention further involves a method of determining three dimensional structures of BACE homologues of unknown structure by using the structural co-ordinates of Table 5. For example, if X-ray crystallographic or NMR spectroscopic data is provided for a BACE homologue of unknown structure, the structure of BACE as defined in Table 5 may be used to interpret that data to provide a likely structure for the BACE homologue by techniques well known in the art, e.g., by phase modeling in the case of X-ray crystallography. Thus, an inventive method can comprise: aligning a representation of an amino acid sequence of a BACE homologue of unknown structure with the amino acid sequence of BACE to match homologous regions of the amino acid sequences; modeling the structure of the matched homologous regions of the BACE of unknown structure on the structure as defined in Table 5 of the corresponding regions of BACE; and, determining a conformation (e.g. so that favorable interactions are formed within the BACE of unknown structure and/or so that a low energy conformation is formed) for the BACE of unknown structure which substantially preserves the structure of said matched homologous regions. "Homologous regions" describes amino acid residues in two sequences that are identical or have similar, e.g., aliphatic, aromatic, polar, negatively charged, or positively charged, side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those skilled in the art. Advantageously, the first and third steps are performed by computer modeling. Homology modeling is a technique that is well known to those skilled in the art (see, e.g., Greer, Science vol. 228 (1985) 1055, and Blundell et al. Eur J Biochem vol 172 (1988), 513).

In general, comparison of amino acid sequences is accomplished by aligning an amino acid sequence of a polypeptide of a known structure with the amino acid sequence of a the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous are grouped together. This method detects conserved regions of the polypeptides and accounts for amino acid insertions and deletions. Homology between amino acid sequences can be determined by using commercially available algorithms. In addition to those otherwise mentioned herein, mention is made too of the programs BLAST, gapped BLAST, BLASTN, and PSI-BLAST, provided by the National Center for Biotechnology Information. These programs are widely used in the art for this purpose and can align homologous regions of two amino acid sequences.

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Once the amino acid sequence of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure. The structures of amino acids located in non-conserved regions may be assigned manually using standard peptide geometries or by molecular simulation techniques, such as molecular dynamics. Refining the entire structure can be by molecular dynamics and/or energy minimization.

The aspects of the invention which employ the BACE structure *in silico* may be equally applied to homologue models of BACE obtained by the above aspect of the invention and this forms yet a further embodiment of the invention. Thus, having determined a conformation of a BACE by the methods described herein, such a conformation may be used in a computer-based method of rational drug or compound design or identification as described herein.

The invention further provides a method for determining the structure of a modulator of BACE bound to BACE comprising: providing a crystal of BACE, e.g., according to the invention, soaking the crystal with the modulator, and determining the structure of the BACE-modulator complex. Alternatively or additionally the BACE and the modulator may be co-crystallized.

Having obtained and characterized a modulator according to the invention, the invention further provides a method for modulating the activity of BACE which comprises: providing BACE under conditions where, in the absence of a modulator, BACE is able to exhibit secretase activity,

providing a modulator compound (e.g., contacting the modulator and the BACE), determining the extent to which the activity of BACE is altered by the presence of the modulator compound.

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The invention further provides systems, such as computer systems, intended to generate structures and/or perform rational drug design for a BACE or complex of BACE and a potential modulator. The system can contain: atomic co-ordinate data according to Table 5 or derived therefrom by homology modeling, said data defining the three-dimensional structure of a BACE or at least one sub-domain thereof; or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5. The invention also involves computer readable media with: atomic co-ordinate data according to Table 5 or derived therefrom by homology modeling, said data defining the three-dimensional structure of a BACE or at least one sub-domain thereof; or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5. "Computer readable media" refers to any media which can be read and accessed directly by a computer, and includes, but is not limited to: magnetic storage media such as floppy discs, hard storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories, such as magnetic/optical media. By providing such computer readable media, the atomic co-ordinate data can be routinely accessed to model BACE or a subdomain thereof. For example RASMOL (Sayle et al., TIBS vol. 20 (1995), 374) is a publicly available software package which allows access and analysis of atomic co-ordinate data for structural determination and/or rational drug design. The invention further comprehends methods of doing business by providing access to such computer readable media and/or computer systems and/or atomic co-ordinate data to users; e.g., the media and/or atomic co-ordinate data can be accessible to a user, for instance on a subscription basis, via the Internet or a global communication/computer network; or, the computer system can be available to a user, on a subscription basis. Structure factor data, which are derivable from atomic co-ordinate data (see, e.g., Blundell et al., in Protein Crystallography, Academic Press, NY, London and San Francisco (1976)), are particularly useful for calculating, e.g., difference Fourier electron density maps. Thus, there are additional uses for the computer readable media and/or computer systems and/or atomic co-ordinate data and additional reasons to provide them to users. A "computer system" refers to the hardware means, software means and data storage means used to analyze the atomic co-ordinate data of the present invention. The minimum hardware means of computer-based

systems of the invention may comprise a central processing unit (CPU), input means, output means, and data storage means. Desirably, a monitor is provided to visualize structure data. The data storage means may be RAM or other means for accessing computer readable media of the invention. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based, Windows NT or IBM OS/2 operating systems.

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The invention also provides a method of analyzing a complex of BACE and a potential modulator comprising: employing X-ray crystallographic diffraction data from the complex and a three-dimensional structure of BACE or at least a sub-domain thereof, to generate a difference Fourier electron density map of the complex; advantageously, the three-dimensional structure being as defined by the atomic co-ordinate data according to Table 5.

Such complexes can be crystallized and analyzed using X-ray diffraction methods, e.g., according to the approaches described by Greer et al., J of Medicinal Chemistry, vol 37 (1994), 1035-54, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallized BACE and the solved structure of uncomplexed BACE. These maps can then be used to determine whether and where a particular potential modulator binds to BACE and/or changes the conformation of BACE. Electron density maps can be calculated using programs such as those from the CCP4 computer package (Collaborative Computing Project, No. 4. The CCP4 Suite: Programs for Protein Crystallography, Acta Crystallographica, D50, 1994, 760-763). For map visualization and model building programs such as "QUANTA" (1994, San Diego, CA: Molecular Simulations, Jones et al., Acta Crystallography A47 (1991), 110-119) can be used.

Table 5 gives atomic co-ordinate data for BACE complexed with OM99-2, and lists each atom by a unique number; the chemical element and its position in each amino acid residue, the amino acid residue in which the element is located, the chain identifier, the number of the residue, co-ordinates (e.g., X, Y, Z) which define with respect to the crystallographic axes the atomic position (in Å) of the respective atom, the occupancy of the atom in the respective position, "B", isotropic displacement parameter (in Å²) which accounts for movement of the atom around its atomic center, and atomic number.

Determination of the 3D structure of BACE provides important information about the likely active site(s) of BACE, particularly when comparisons are made with other enzymes, such as

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similar enzymes. This information may be used for rational design of BACE inhibitors, e.g., by computational techniques that identify possible binding ligands for the active site(s), by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands using analyses such as X-ray crystallographic analysis.

Greer et al., *supra*, relates to an iterative approach to ligand design based on repeated sequences of computer modeling, protein-ligand complex formation, and X-ray analysis. Thymidylate synthase inhibitors were designed by Greer; and, BACE inhibitors may also be designed in this way. Using, for example, GRID (P. Goodford, J. Med. Chem, 1985, 28, 849-57) or the solved 3D structure of BACE, a potential modulator of BACE may be designed that complements the functionalities of the BACE active site(s). The potential modulator can be synthesized, formed into a complex with BACE, and the complex then analyzed, e.g., by X-ray crystallography, NMR or a combination thereof, to identify the actual position of the bound compound.

Determination of the position of the potential modulator compound in the complex allows determination of the interactions of it with BACE. This allows the skilled artisan to analyze the affinity and specificity of the compound for BACE, and to propose modifications to the compound to increase or decrease either or both of these properties. Thus, the structure and/or functional groups of the compound can then be adjusted, if necessary or desired, in view of the results from the analysis (e.g., X-ray analysis), and the synthesis and analysis sequence repeated until an optimized compound is obtained. Related approaches to structure-based drug design are also discussed in other documents cited herein, as well as in Bohacek et al., Medicinal Research Reviews, vol. 16 (1996), 3-5.

As a result of the determination of the BACE 3D structure, more purely computational techniques for rational drug design may also be used to design BACE modulators; for example, automated ligand-receptor docking programs (see Jones et al., in Current Opinion in Biotechnology, vol 6 (1995), 652-656) which require accurate information on the atomic coordinates of target receptors, may be used to design or identify potential BACE modulators or inhibitors.

Linked-fragment approaches to drug design also require accurate information on the atomic co-ordinates of a target. Small compounds that have the potential to bind to regions of BACE which in themselves may not be modulator compounds may be assembled by chemical linkage to

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provide potential modulators. Thus, the basic idea behind these approaches is to determine the binding locations of more than one, e.g., plural or a plurality of, ligands to a target molecule, and then construct a molecular scaffold to connect the ligands together in such a way that their relative binding positions are preserved. The ligands may be provided computationally and modeled in a computer system, or provided in an experimental setting, wherein crystals according to the invention are provided and more than one, e.g., plural or a plurality of, ligands soaked separately or in mixed pools into the crystal prior to analysis, e.g., X-ray analysis, and determination of their location.

The binding site of two or more ligands are determined and may be connected to thus form a potential lead compund that can be further refined, e.g., the iterative technique of Greer et al. For a virtual linked-fragment approach, see Verlinde et al., J of Computer-Aided Molecular Design 6 (1992), 131-147 and for NMR and X-ray approaches, see Skuker et al., Science 274 (1996), 1531-1534, and Stout et al., Structure 6 (1998), 839-48. The use of these or other approaches to design and/or identify BACE modulators (see, e.g., patent documents cited herein such as in the Background Section, supra) is made possible by the determination of the BACE structure.

Many of the techniques and approaches to structure-based described herein employ X-ray analysis to identify the binding position of a potential modulator in a complex with a protein. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the potential modulator. However, to produce a map (See Blundell et al., supra), it is important to know the 3D structure of the protein beforehand (or at least the protein structure factors). Therefore, determination of the BACE structure also allows difference Fourier electron density maps of complexes of BACE with a potential modulator to be produced, which can greatly assist in the process of rational compound and/or drug design or identification.

The approaches to structure-based drug or compound design or identification described herein involve initial identification of possible compounds for interaction with the target molecule (in this case BACE). Sometimes these compounds are known, e.g., from research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug or compound design or identification program may involve computer-based *in silico* screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the active site or sites of the target bio-molecule (in this case

BACE). Screening selection criteria may be based on pharmacokinetic properties such as metabolic stability and toxicity. However, determination of the BACE structure allows the architecture and chemical nature of each BACE active site to be identified, which in turn allows the geometric and functional constraints of a descriptor for the potential inhibitor to be derived. The descriptor can be, therefore, a type of virtual 3D pharmacophore, which can also be used as selection criteria or filter for database screening.

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Compounds which have a chemical structure selected using the invention, wherein said compounds are BACE modulators or inhibitors, form a further aspect of the invention; and, such compounds may be used in methods of medical treatments, such as for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies involving BACE or the production of $A\beta$ or fragments thereof. Further, such compounds may be used in the preparation of medicaments for such treatments. The compounds may be employed alone or in combination with other treatments for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies involving BACE or the production of $A\beta$ or fragments thereof; and, the compounds may be used in the preparation of combination medicaments for such treatments, or in kits containing the compound and the other treatment.

Turning more specifically to BACE, BACE is a pepsin-like aspartyl proteinase, the mature enzyme consisting of the N-terminal catalytic domain, a transmembrane domain, and a small cytoplasmic domain. BACE has an optimum activity at pH 4.5 (Vassar et al., 1999) or pH 5.0 (Yan et al. 1999) and is found in acidic subcellular compartments such as golgi and endosomes (Vassar et al., 1999 and Capell et al., 2000). The pH in the endosome and trans golgi network, where BACE appears to function, fluctuates in the range of pH 4.5 - 6.0 with the average pH being stated as 5.0 (Lee et al. 1996) and pH 5.4 (Overly et al. 1995). BACE is not inhibited by standard pepsin inhibitors such as pepstatin. It has been shown that the catalytic domain minus the transmembrane and cytoplasmic domain has activity against substrate peptides (Lin et al, 2000). Consequently, this soluble catalytic domain is suitable for crystallization studies and a crystal structure of this will give a representative structure of the BACE active site for the design of inhibitor molecules. Ideally it would be desirable to crystallize a form of BACE with an unoccupied active site. This could be used to soak in small molecule inhibitors of the enzyme and to investigate their binding modes. Crystals of BACE grown both in the presence and absence of inhibitor, having same space group and similar unit cell parameters are described. These crystals are grown between pH 5.6 and

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pH 5.8 and thus are grown at the biologically relevant pH of BACE. This is also close to the optimum pH of the enzyme. Upon soaking the C2 crystal form with a ligand, some reorganization of the molecules in the crystal will take place, resulting in a space group change from C2 to P2₁. The cell dimensions and the packing of the P2₁ form are closely related to those of the C2 form. Because the BACE crystals are grown at physiologically relevant pH the compounds identified in accordance with the invention would be of more biological relevance. The lead compounds/inhibitors generated may be of higher therapeutic value and would truly reflect the mode of inhibition *in vivo*, particularly for those compounds that are susceptible to changes in protonation state.

A synthetic gene encoding the pro- and aspartyl protease domains of BACE was constructed (see Example 1). The construct extended from Thr 22 to Ser 453 (numbering refers to the full-length BACE sequence, e.g. Genbank accession P56817, SEQ ID NO:6). In each of the four potential glycosylation sites (Asn-X-Ser/Thr: Asparagines-153, -172, -223 and -354) the Asparagine residue was mutated to Glutamine to prevent glycosylation of the protein. Silent mutations were also introduced into the coding sequence in order to reduce the GC content of the gene (Figure 1A shows an alignment of the synthetic DNA sequence of the present invention with other wild-type BACE genes). A His6 peptide tag was added to the C-terminus of the protein sequence to facilitate purification on Nickel agarose (see Example 1).

Both forms of the protein could be detected using an anti-His6 antibody (see Figure 5); only the unprocessed form containing the pro-peptide was detected using an anti-FLAG antibody. Further changes to the synthetic BACE catalytic domain sequence were the addition of the baculoviral gp67 signal sequence instead of the BACE signal, the addition of a FLAG tag to the N-terminus of the pro-peptide. The gp67 signal sequence increased the secretion of the protein into the cell culture medium, and the FLAG tag was added to allow differentiation between species arising from incomplete pro-peptide cleavage (and to determine if separation is required) (see Figure 6). Insect cells infected with the BACE baculovirus secreted a mixture of processed and unprocessed BACE into the culture medium. Figure 2A shows the polypeptide sequence encoded by the synthetic BACE gene.

As mentioned previously, the invention comprehends the use of the inventive BACE proteins in assays or methods for determining inhibitors thereof, e.g., compounds, compositions or active agents or ingredients that bind to BACE, advantageously irreversibly, preferably so as to

have a therapeutic effect with respect to AD and other maladies. After determination of a suitable compound, composition, active agent or ingredient that binds to BACE, the compound, composition, active agent or ingredient is then formulated into a composition for administration and is administered to a subject in need thereof. These therapeutics can be administered in known formulations, by known routes of administration, following the teachings of documents cited herein.

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It is noted that these therapeutics can be a chemical compound and/or antibody and/or portion thereof or a pharmaceutically acceptable salt and can be administered alone or as an active ingredient in combination with pharmaceutically acceptable carriers, diluents, and vehicles, as well as other active ingredients.

The compounds can be administered orally, subcutaneously or parenterally including intravenous, intraarterial, intramuscular, intraperitoneally, and intranasal administration as well as intrathecal and infusion techniques.

It is noted that humans are treated generally longer than the mice or other experimental animals which treatment has a length proportional to the length of the disease process and drug effectiveness. The doses may be single doses or multiple doses over a period of several days, but single doses are preferred. Thus, one can scale up from animal experiments, e.g., rats, mice, and the like, to humans, by techniques from this disclosure and documents cited herein and the knowledge in the art, without undue experimentation.

The treatment generally has a length proportional to the length of the disease process and drug effectiveness and the patient being treated.

When administering a therapeutic of the present invention parenterally, it will generally be formulated in a unit dosage injectable form (solution, suspension, emulsion). The pharmaceutical formulations suitable for injection include sterile aqueous solutions or dispersions and sterile powders for reconstitution into sterile injectable solutions or dispersions. The carrier can be a solvent or dispersing medium containing, for example, water, ethanol, polyol (for example, glycerol, propylene glycol, liquid polyethylene glycol, and the like), suitable mixtures thereof, and vegetable oils.

Proper fluidity can be maintained, for example, by the use of a coating such as lecithin, by the maintenance of the required particle size in the case of dispersion and by the use of surfactants. Nonaqueous vehicles such a cottonseed oil, sesame oil, olive oil, soybean oil, corn oil, sunflower

oil, or peanut oil and esters, such as isopropyl myristate, may also be used as solvent systems for compound compositions

Additionally, various additives which enhance the stability, sterility, and isotonicity of the compositions, including antimicrobial preservatives, antioxidants, chelating agents, and buffers, can be added. Prevention of the action of microorganisms can be ensured by various antibacterial and antifungal agents, for example, parabens, chlorobutanol, phenol, sorbic acid, and the like. In many cases, it will be desirable to include isotonic agents, for example, sugars, sodium chloride, and the like. Prolonged absorption of the injectable pharmaceutical form can be brought about by the use of agents delaying absorption, for example, aluminum monostearate and gelatin. According to the present invention, however, any vehicle, diluent, or additive used would have to be compatible with the compounds.

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Sterile injectable solutions can be prepared by incorporating the compounds utilized in practicing the present invention in the required amount of the appropriate solvent with various amounts of the other ingredients, as desired.

A pharmacological formulation of the present invention, e.g., comprising a therapeutic compound, can be administered to the patient in an injectable formulation containing any compatible carrier, such as various vehicles, adjuvants, additives, and diluents; or the compounds utilized in the present invention can be administered parenterally to the patient in the form of slow-release subcutaneous implants or targeted delivery systems such as monoclonal antibodies, iontophoretic, polymer matrices, liposomes, and microspheres.

A pharmacological formulation of the compound utilized in the present invention can be administered orally to the patient. Conventional methods such as administering the compounds in tablets, suspensions, solutions, emulsions, capsules, powders, syrups and the like are usable. Known techniques which deliver the compound orally or intravenously and retain the biological activity are preferred.

In one embodiment, a formulation of the present invention can be administered initially, and thereafter maintained by further administration. For instance, a formulation of the invention can be administered in one type of composition and thereafter further administered in a different or the same type of composition. For example, a formulation of the invention can be administered by intravenous injection to bring blood levels to a suitable level. The patient's levels are then

maintained by an oral dosage form, although other forms of administration, dependent upon the patient's condition, can be used.

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The quantity to be administered will vary for the patient being treated and will vary from about 100 ng/kg of body weight to 100 mg/kg of body weight per day and preferably will be from 10 pg/kg to 10 mg/kg per day. For instance, dosages can be readily ascertained by those skilled in the art from this disclosure and the knowledge in the art. Thus, the skilled artisan can readily determine the amount of compound and optional additives, vehicles, and/or carrier in compositions and to be administered in methods of the invention. Typically, an adjuvant or additive is commonly used as 0.001 to 50 wt% solution in phosphate buffered saline, and the active ingredient is present in the order of micrograms to milligrams, such as about 0.0001 to about 5 wt%, preferably about 0.0001 to about 1 wt%, most preferably about 0.0001 to about 0.05 wt% or about 0.001 to about 20 wt%, preferably about 0.01 to about 10 wt%, and most preferably about 0.05 to about 5 wt%. Of course, for any composition to be administered to an animal or human, and for any particular method of administration, it is preferred to determine therefor: toxicity, such as by determining the lethal dose (LD) and LD₅₀ in a suitable animal model e.g., rodent such as mouse; and, the dosage of the composition(s), concentration of components therein and timing of administering the composition(s), which elicit a suitable response, such as by titrations of sera and analysis thereof. Such determinations do not require undue experimentation from the knowledge of the skilled artisan, this disclosure and the documents cited herein. And, the time for sequential administrations can be ascertained without undue experimentation.

Examples of compositions comprising a therapeutic of the invention include liquid preparations for orifice, e.g., oral, nasal, anal, vaginal, peroral, intragastric, mucosal (e.g., perlingual, alveolar, gingival, olfactory or respiratory mucosa) etc., administration such as suspensions, syrups or elixirs; and, preparations for parenteral, subcutaneous, intradermal, intramuscular or intravenous administration (e.g., injectable administration), such as sterile suspensions or emulsions. Such compositions may be in admixture with a suitable carrier, diluent, or excipient such as sterile water, physiological saline, glucose or the like. The compositions can also be lyophilized. The compositions can contain auxiliary substances such as wetting or emulsifying agents, pH buffering agents, gelling or viscosity enhancing additives, preservatives, flavoring agents, colors, and the like, depending upon the route of administration and the preparation desired. Standard texts, such as "REMINGTON'S PHARMACEUTICAL SCIENCE",

17th edition, 1985, incorporated herein by reference, may be consulted to prepare suitable preparations, without undue experimentation.

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Compositions of the invention, are conveniently provided as liquid preparations, e.g., isotonic aqueous solutions, suspensions, emulsions or viscous compositions which may be buffered to a selected pH. If digestive tract absorption is preferred, compositions of the invention can be in the "solid" form of pills, tablets, capsules, caplets and the like, including "solid" preparations which are time-released or which have a liquid filling, e.g., gelatin covered liquid, whereby the gelatin is dissolved in the stomach for delivery to the gut. If nasal or respiratory (mucosal) administration is desired, compositions may be in a form and dispensed by a squeeze spray dispenser, pump dispenser or aerosol dispenser. Aerosols are usually under pressure by means of a hydrocarbon. Pump dispensers can preferably dispense a metered dose or, a dose having a particular particle size.

Compositions of the invention can contain pharmaceutically acceptable flavors and/or colors for rendering them more appealing, especially if they are administered orally. The viscous compositions may be in the form of gels, lotions, ointments, creams and the like (e.g., for transdermal administration) and will typically contain a sufficient amount of a thickening agent so that the viscosity is from about 2500 to 6500 cps, although more viscous compositions, even up to 10,000 cps may be employed. Viscous compositions have a viscosity preferably of 2500 to 5000 cps, since above that range they become more difficult to administer. However, above that range, the compositions can approach solid or gelatin forms which are then easily administered as a swallowed pill for oral ingestion.

Liquid preparations are normally easier to prepare than gels, other viscous compositions, and solid compositions. Additionally, liquid compositions are somewhat more convenient to administer, especially by injection or orally. Viscous compositions, on the other hand, can be formulated within the appropriate viscosity range to provide longer contact periods with mucosa, such as the lining of the stomach or nasal mucosa.

Obviously, the choice of suitable carriers and other additives will depend on the exact route of administration and the nature of the particular dosage form, e.g., liquid dosage form (e.g., whether the composition is to be formulated into a solution, a suspension, gel or another liquid form), or solid dosage form (e.g., whether the composition is to be formulated into a pill, tablet, capsule, caplet, time release form or liquid-filled form).

Solutions, suspensions and gels, normally contain a major amount of water (preferably purified water) in addition to the active compound. Minor amounts of other ingredients such as pH adjusters (e.g., a base such as NaOH), emulsifiers or dispersing agents, buffering agents, preservatives, wetting agents, jelling agents, (e.g., methylcellulose), colors and/or flavors may also be present. The compositions can be isotonic, i.e., it can have the same osmotic pressure as blood

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and lacrimal fluid.

The desired isotonicity of the compositions of this invention may be accomplished using sodium chloride, or other pharmaceutically acceptable agents such as dextrose, boric acid, sodium tartrate, propylene glycol or other inorganic or organic solutes. Sodium chloride is preferred particularly for buffers containing sodium ions.

Viscosity of the compositions may be maintained at the selected level using a pharmaceutically acceptable thickening agent. Methylcellulose is preferred because it is readily and economically available and is easy to work with. Other suitable thickening agents include, for example, xanthan gum, carboxymethyl cellulose, hydroxypropyl cellulose, carbomer, and the like. The preferred concentration of the thickener will depend upon the agent selected. The important point is to use an amount which will achieve the selected viscosity. Viscous compositions are normally prepared from solutions by the addition of such thickening agents.

A pharmaceutically acceptable preservative can be employed to increase the shelf-life of the compositions. Benzyl alcohol may be suitable, although a variety of preservatives including, for example, parabens, thimerosal, chlorobutanol, or benzalkonium chloride may also be employed. A suitable concentration of the preservative will be from 0.02% to 2% based on the total weight although there may be appreciable variation depending upon the agent selected.

Those skilled in the art will recognize that the components of the compositions should be selected to be chemically inert with respect to the active compound. This will present no problem to those skilled in chemical and pharmaceutical principles, or problems can be readily avoided by reference to standard texts or by simple experiments (not involving undue experimentation), from this disclosure and the documents cited herein.

The inventive compositions of this invention are prepared by mixing the ingredients following generally accepted procedures. For example the selected components may be simply mixed in a blender, or other standard device to produce a concentrated mixture which may then be adjusted to the final concentration and viscosity by the addition of water or thickening agent and

possibly a buffer to control pH or an additional solute to control tonicity. Generally the pH may be from about 3 to 7.5. Compositions can be administered in dosages and by techniques well known to those skilled in the medical and veterinary arts taking into consideration such factors as the age, sex, weight, and condition of the particular patient, and the composition form used for administration (e.g., solid vs. liquid). Dosages for humans or other mammals can be determined without undue experimentation by the skilled artisan, from this disclosure, the documents cited herein, and the knowledge in the art.

Suitable regimes for initial administration and further doses or for sequential administrations also are variable, may include an initial administration followed by subsequent administrations; but nonetheless, may be ascertained by the skilled artisan, from this disclosure, the documents cited herein, and the knowledge in the art.

Accordingly, the invention comprehends, in further aspects, methods for preparing therapeutic compositions including an active agent, ingredient or compound or BACE inhibitor as from inventive methods herein for ascertaining compounds that bind to and/or inhibit BACE, as well as to methods for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD or other maladies.

Furthermore, as discussed herein, the inventive BACE proteins are useful in generating antibodies, which are themselves useful in assays as well as in therapeutics. From documents cited herein, one can readily make and use anti-BACE antibodies and methods for producing monoclonal antibodies are well known to those of ordinary skill in the art, see, e.g., U.S. Patent No. 4,196,265 and 6,221,645. Thus, the BACE proteins of the invention can be used to generate antibodies and the antibodies can be used, without undue experimentation.

The invention will now be further described by the following non-limiting Examples, given by way of illustration.

EXAMPLES

EXAMPLE 1: Production of BACE in Insect Cells

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A. Gene Construction and Cloning

The synthetic BACE catalytic domain sequence was constructed a combination of oligonucleotide synthesis and overlap PCR (Cambridge Bioscience Ltd, Cambridge UK).

Mutations were inserted at specific sites within the BACE catalytic domain sequence during synthesis to reduce the GC content of the gene. The synthetic gene was then cut with restriction

enzymes Sal1 and Not1 to generate a 1489 bp fragment which was then subcloned into the expression vector pFastBac1 (LifeTechnologies), and the DNA sequence verified by standard DNA sequencing methods (e.g., electrophoresis and automated DNA sequence analysis of the insert).

The cDNA encoding human furin was cut by restriction enzymes to generate a 3216 bp Smal Xmal fragment that was then subcloned into the expression vector pFastBac Dual (LifeTechnologies).

B. Baculovirus Generation and Fermentation

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Recombinant baculoviruses were constructed by using the expression vectors of the Bacto-Bac™ system (LifeTechnologies), according to the manufacturers instructions. Manipulations involving insect cells and baculoviruses were carried out according to standard protocols (King and Possee, 1992).

As it has been shown that coexpression of the prohormone convertase furin increases expression of mature TGF-β in insect cells (Laprise et al., 1998), the effect of furin co-expression on BACE production was evaluated i.e., while the total amount of BACE produced did not increase with furin coespression, there was a reproducible increase in the fraction of processed protein from about 30% of total BACE up to about 60%; this result is quite surprising and advantageous.

Trichoplusia ni HighFive cells (Invitrogen, Carlsbad CA,USA) were found to give higher levels of BACE expression than Spodoptera frugiperda Sf9 cells, and were used for all protein production. Protein production was carried out in a 20-30 liter working volume bioreactor (Applikon Dependable Instruments, Schiedam, Netherlands), containing Excell 405 medium (JRH Scientific). Cells were infected at a multiplicity of infection (MOI) of 0.1 of each virus at a cell density of 1.5x106 cells/ml. Glucose concentration was measured during the fermentation and adjusted to maintain the starting concentration. Three days after viral infection the HighFive cells were cleared from the medium by continuous flow centrifugation and the medium was concentrated approximately 30-fold by ultrafiltration.

C. Purification of BACE

The expressed BACE protein was purified by affinity chromatography on nickel agarose resin. Initially, the concentrated medium containing the expressed BACE protein was dialysed overnight against 50mM sodium phosphate pH 8.0, 50mM sodium acetate, 300mM NaCl and 10ml Ni-NTA agarose resin (Qiagen) and equilibrated in the above buffer. Imidazole (Sigma) was added to a final concentration of 5mM, Pefabloc (Roche Molecular Biochemicals, Lewes, UK) was

added to 0.1g/L and the sample was mixed gently overnight at 4°C. The nickel agarose resin was then loaded onto an empty column and washed with 50mM sodium phosphate pH 8.0, 300mM NaCl until the absorption at 280 nm reached the baseline level of the above-mentioned buffer. The column was then washed with 4 column volumes of 50mM sodium phosphate pH 8.0, 50mM NaCl, 15mM imidazole. The BACE protein was then eluted with a linear imidazole concentration gradient, five column volumes in size, from 50mM sodium phosphate pH 8.0, 50mM NaCl to 50mM sodium phosphate pH 8.0, 50mM NaCl, 300mM imidazole, typically resulting in an absorption peak at 280nm, corresponding to the BACE protein and other co-purified contaminating proteins.

After Nickel chromatography the BACE protein was purified by anion exchange chromatography, fractions corresponding to the BACE protein containing the peak were buffer exchanged on a XK-50 column (Amersham Pharmacia Biotech) containing 200 ml sephacryl S-200, into 25 mM Tris pH 8.1, 5mM NaCl (Anion loading buffer) and then loaded onto a Resource Q anion exchange column (Amersham Pharmacia Biotech). The protein was eluted with a 35 column volume linear salt gradient from 100% loading buffer to 100% elution buffer (25mM Tris pH8.1, 400mM NaCl). Fractions were pooled based on analysis by SDS-PAGE.

The pooled fractions were dialysed against HIC loading buffer: 50mM Tris pH 8.1, 50mM NaCl, 0.9 M (NH₄)₂SO₄. The final sample was then loaded onto a HIC column (Source PHE, Amersham Pharmacia Biotech) equilibrated with HIC loading buffer, and washed to a stable baseline with loading buffer. The differentially processed forms of the BACE generated by proteolytic activity were eluted as separate peaks using a 35 column volume gradient from loading buffer to 50mM Tris pH 8.1, 50mM NaCl.

Peak fractions containing the required form of BACE protein were pooled based on analysis by SDS-PAGE and dialysed against 50mM HEPES pH 8.0, 100mM NaCl, 1Mm DTT.

The dialysed sample was concentrated to a 12ml volume and loaded immediately onto a Sephacryl S-200 column (Amersham Pharmacia Biotech) pre-equilibrated with 50mM HEPES pH 8.0, 100mM NaCl, 1 Mm DTT and stored at 4°C after elution.

The purified BACE eluted from the size exclusion column at the position expected for monomeric protein and was monodisperse when subjected to dynamic light scattering. SDS-PAGE showed the representative samples after the different column steps is shown in Figure 5.

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5 **EXAMPLE 2:** Crystallization of BACE

A. Crystallization

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Crystals of BACE were grown by the hanging drop vapor diffusion method, in which 1µl of protein solution and 1µl of well solution (100mM Tri-sodium citrate, pH 5.8, 200mM ammonium iodide and 18-20% PEG monomethyl ether, 5K) were placed on a cover slip and equilibrated over 1ml of well solution at 20°C. The protein concentration was 5mg/ml in 50mM HEPES, pH 8.0, 150mM NaCl, 1mM DTT. Small prismatic crystals appeared after two days and grew to a maximum size of 0.2mm x 0.1mm x 0.1mm after two weeks. (Figures 3A and B).

Crystals of BACE complexed with OM99-2 (Ghosh et al., 2000) were grown using a similar method. BACE, at a concentration of 0.2mg/ml was mixed with an excess of inhibitor and kept at 4°C for 1 hour. The BACE protein was then concentrated to 5mg/ml using a centricon column with a molecular weight cutoff of 10000, and the crystallization drops set up as before. Crystals with the same morphology as the uncomplexed enzyme appeared after two days and grew to a maximum size of 0.25mm x 0.1mm x 0.1mm.

Both BACE with no inhibitor and BACE in the presence of OM99-2 formed crystals belonging to space group C2. The cell dimensions for the crystals grown in the presence of OM99-2 (Figure 3A) were a=236.63Å, b=105.02Å, c=62.59Å and β = 101.32°, and the asymmetric unit of the crystal contained 3 copies of BACE. The cell dimensions for the crystals grown in the absence of any inhibitor (Figure 3B) were a=238.3Å, b=107.4Å, c=60.4Å, b=101.89°.

Apo-Soaked Crystal Experimental: Crystals of BACE, grown in the absence of inhibitor as previously described were soaked in a solution of inhibitor for 1 hour. The inhibitor was previously dissolved in DMSO to a concentration of 10 mM and then diluted 1 in 10 in the well solution as previously described. 20 microliters of this was placed in a microbridge, and an apo BACE crystal added to it. The microbridge was sealed and incubated for 3.5 hours.

B. Data collection and processing

The structure of BACE as a complex with OM99-2 was solved to 2.6Å using the method of molecular replacement. Data was collected at 100K on crystals frozen in a solution containing a suitable cryoprotectant. The cryoprotectant solution consisted of 100mM Tri-sodium citrate, pH 5.8, 200mM ammonium iodide, 15% PEG monomethyl ether 5K, and 20% PEG 400. The crystal was immersed in the cryoprotectant solution for 30 seconds prior to freezing in liquid nitrogen for the purposes of storage. Data was collected to 2.6Å on beamline ID14-2 at the European

Synchrotron Radiation Facility using a MARCCD detector, with a wavelength of 0.934A and processed using D*trek (Pflugrath, J., 1999). The dataset was scaled using SCALA and the intensities converted to structure factors using TRUNCATE, from the CCP4 suite of programs (Collaborative Computing Project, 1994). Statistics for the processed data are listed in Table 1.

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TABLE 1: Data collection statistics for BACE crystallized as a complex with OM99-2.

<u> </u>	2.6Å
Resolution	2.0A
Mosaicity	0.8°
Completeness	95.4%
Multiplicity	1.96
Rmerge	0.087

This table shows that the experimental data used to solve the structure of the BACE/OM99-2 complex was of good quality and sufficient completeness to enable a reliable structure to be derived from it.

Apo-Crystal Experimental: The soaked crystal was then removed, dipped in a solution containing a cryoprotectant mixed with the inhibitor in DMSO, in the same proportions as previously (100 mM Tri-sodium citrate, pH 5.8, 200 mM ammonium iodide, 15% PEG monomethyl ether 5K and 20% PEG 400). The crystal was then frozen as for the OM99-2 crystals and data collected. Data was collected on station ID14-1 at the ESRF using an ADSC detector.

C. Structure Determination and Refinement

The structure of the BACE/OM99-2 complex was solved by molecular replacement using the program AMORE (Navaza, 1994). The molecular replacement solution was not as straightforward application of AMORE. Rather, it involved the use of CCP4, the programs POLARRFN and RFCORR, as well as inventive effort, e.g., to so use this combination and especially to so use RFCORR (Collaborative Computing Project, 1994). The search model was the A chain of 1FKN (Hong et al. 2000) taken from the pdb database (1FKN.pdb); a search radius of 35Å and a resolution range of 8.0-3.0Å being used to give a solution with an Rfactor of 0.38 and a

correlation coefficient of 0.714. This solution was used as a starting point for refinement using the program REFMAC5, also from the CCP4 suite of programs (Collaborative Computing Project, 1994). The inhibitor, OM99-2 was absent from the initial model, and convincing electron density in the active site of all three copies of BACE was observed in difference Fourier maps. This provided confirmation that the solution to the molecular replacement was correct. Cycles of refinement of the structure were alternated with manual rebuilding of the model using QUANTA (1994, San Diego, CA: Molecular Simulations). The N- and C- termini of the molecule were rebuilt, asparagine residues 153, 172, 223 and 354 were remodeled as glutamine residues. The inhibitor molecule was built into the electron density with QUANTA (1994, San Diego, CA: Molecular Simulations), and finally the water molecules were added using DenInt (Astex internal software library). Refinement statistics are shown in Table 2A.

Data collected with apo crystals soaked with inhibitor were processed using D*Trek (Pflugrath, J., 1999), and the intensities converted to structure factors using TRUNCATE, from the CCP4 suite of programs (Collaborative Computing Project, 1994).

The space group of these crystals has changed from the apo form (space group C2) to P2₁ with cell dimensions a=62.8, b=106.8Å, c=227.9Å and β =93.63°. The statistics are given in Table 2B below

The structure of the soaked BACE/inhibitor complex was solved by molecular replacement using the programs AMORE (Navaza, 1994). The search model was a monomer from the BACE/OM99-2 structure. A search radius of 35 Å and a resolution range of 12 – 4Å gave a solution with and Rfactor of 0.421 and a correlation coefficient of 0.638. There are 6 monomers in the asymmetric unit. This solution was used as a starting point for refinement using the programs CNX (1999, San Diego, CA: Molecular Simulations) and BUSTER (Bricogne, 1993, Acta Cryst. D49, 37-60). The final refinement statistics are given in Table 2C below.

TABLE 2A: Final refinement statistics for The C2 BACE/OM99-2 complex.

Rwork	0.231	
Rfree	0.312	
RMS bond deviation from ideality	0.022Å	
RMS bond angle deviation from ideality	2.4°	= 8 =
Average Bfactor for structure	53.4Å ²	

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This data indicates that the final structure is of good quality, the Rfactors indicating that the refined model has a good agreement with the experimental data. The RMS deviations from ideality indicate that the geometry of the model is good and in agreement with previous data.

TABLE 2B: Statistics for P2₁ BACE/inhibitor complex

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Resolution	3.0 Å
Mosaicity	0.45
Completeness	98%
Multiplicity	2.3
Rmerge	13.8%

The statistics show the space group has changed from the apo-BACE form (space group C2) to P2₁ with cell dimensions a=62.8, b=106.8Å, c=227.9Å and β=93.63°

TABLE 2C: Final refinement statistics for P2₁ BACE/inhibitor complex.

Rwork	30.3%	
Rfree	34.5%	
RMS bond deviation from ideality	0.015 Å	
RMS bond angle deviation from ideality	1.027°	·
Average Bfactor for structure	35.6 Å	

RESULTS AND DISCUSSION

The final model of the C2 crystal structure of BACE/OM99-2 contained 1161 residues in 3 protein molecules, 3 copies of OM99-2 and 183 ordered water molecules, an Rfactor of 0.231 and a free Rfactor of 0.312. The asymmetric unit contained 3 copies of the BACE molecule (Figures 4A and B), A, B and C, two of which, B and C, form a dimer related by a non-crystallographic two-fold axis. Molecule A forms a similar dimer with its crystallographically related molecule A in an adjacent asymmetric unit. The positions of residues –2 to 385 of all three independent molecules are well defined by the electron density. There is no evidence of density beyond serine –2 for any of the molecules, and the N-terminus of molecules A and C interact with OD1 of asparagine 98 in symmetry related molecules B and A respectively. The N-terminus of molecule B is in a region of solvent. This lack of electron density for all three molecules indicates that the other residues from the N-terminus have no ordered structure. The electron density at the C-terminus ends with residue Asn 385, with no evidence for further terminal residues for the His-tag.

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The bilobal structure of individual molecules of BACE as solved in the C2 crystal form, is essentially the same as that of memapsin 2 as solved in the P2₁ crystal form. The interactions made by the specific mutations are shown in Table 3. These include the N and C-terminus and the Asn \rightarrow Gln mutations in each of the three independent units. The mutation of Asn111 to Gln111 appears to be important in the formation of the crystals in that Gln111 of molecule B lies close to the crystallographic two-fold axis and interacts with the symmetry related B:111. Difference electron density was initially seen for OM99-2 in all three molecules, and the inhibitor molecule was fitted to this. Its position was well defined from P4 to P4' for molecules A and C P4' was less well defined in molecule B. The active site is open to solvent for molecules B and C, but that of molecule A is partially occluded (close to P4') by a symmetry related molecule C.

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TABLE 3: Interactions made by mutated residues in BACE. Monomers AB and C are described in column 1 and the residues with which they interact in column 2.

Mutated or different residue (from	Interactions formed by mutated or different
Tang sequence)	residue.
A:92	B:142, a crystallographic symmetry related lysine
A:111	No direct interactions
A:162	No direct interactions
A:293	No direct interactions
B:92	No direct interactions
B:111	B:111 symmetry related glutamine, lies on 2-fold
B:162	Close to crystallographic symmetry axis, but no
·	direct interactions
B:293	Points towards solvent channel
C:92	A:142 a crystallographic symmetry related lysine
C:111	No direct interactions
C:162	No direct interactions
C:293	No direct interactions
A:Nterm	Nterm makes interaction with symmetry related
	OD1 of Asn98B
B:Nterm	Nothing beyond residue ser-2
C:Nterm	N-term makes interaction with symmetry related
	OD1 of Asn98A
A:Cterm	No interactions
B:Cterm	No interactions
C:Cterm	No interactions.

This table shows that most of the mutations made to the BACE enzyme are at positions which do not affect the crystal packing. The major exception is in the case of residue B111, which is shown to interact across the crystallographic two-fold axis with its symmetry related molecule.

5 TABLE 4: Comparison of Tang/Hong structure with present invention.

Measurement	Tang /Hong	Present Invention
Inhibitor OM99-2	Crystallized in presence of	Crystallized in presence and
	inhibitor OM99-2	absence of OM99-2.
Crystallisation conditions	5mg/ml protein, 5-fold molar	6mg/ml protein, excess
	excess of OM99-2	OM99-2, 0.2M ammonium
	0.2M ammonium sulphate,22.5%	iodide, 20% PEGMME5K,
e	PEG8K, 0.1M Na-cacodylate,	0.1M tri-sodium citrate, pH
	pH 7.4	5.6-5.8
Space Group	P2 ₁	C2
Cell dimensions(Å)	a=53.7,b=85.9,109.2,beta=101.4°	a=236.6,b=105.0,c=62.59,
		beta=101.3°
Resolution	1.9Å	2.6Å
pH of crystallization	7.4	5.8
Molecules in asymmetric	2	3
unit		
N-terminus	-28p	-33p
C-terminus	No His-tag	His-tag
Mutations	None known	Asn→Gln (glycosylation
		sites)
Dimer interface	Around N209	Same dimer interface
B:111 environment	solvent exposed	interact across 2-fold axis.
Accessibility of active site	Both molecules accessible	1 accessible, 1 inaccessible,
		1 partly accessible
OM99-2 binding mode	As described in Science, 2000	Binding modes similar, but
	290 150-153	P4' is more ordered.

This further demonstrates that the present invention is novel, nonobvious and inventive over the Tang PCT publications and the Hong Science article.

The following Table 5 provides atomic co-ordinates of BACE.

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Table 5: Atomic co-ordinates.
                                                        XX-XXX-XX
                                                                     XXXX
               ----
    HEADER
     COMPND
     REMARK
              3 REFINEMENT.
     REMARK
                  PROGRAM : REFMAC 5.0
     REMARK
10
     REMARK
     REMARK
                   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
     REMARK 3
             3 DATA USED IN REFINEMENT.
    -REMARK
             3 RESOLUTION RANGE HIGH (ANGSTROMS): 2.60
     REMARK
                  RESOLUTION RANGE LOW (ANGSTROMS): 119.52
     REMARK
                  DATA CUTOFF (SIGMA(F)): NONE
     REMARK
              3 COMPLETENESS FOR RANGE (%): 93.40
     REMARK
              3 NUMBER OF REFLECTIONS
20 REMARK
     REMARK
             3 FIT TO DATA USED IN REFINEMENT.
     REMARK
            3 CROSS-VALIDATION METHOD : THROUGHOUT
3 FREE R VALUE TEST SET SELECTION : RANDOM
3 R VALUE (WORKING + TEST SET) : 0.23480
     REMARK
     REMARK
     REMARK
25
                             (WORKING SET) : 0.23064
            3 R VALUE
     REMARK
                                             : 0.31230
                  FREE R VALUE
     REMARK 3
                  FREE R VALUE TEST SET SIZE (%): 5.1
FREE R VALUE TEST SET COUNT : 2184
     REMARK 3
     REMARK
30
     REMARK
                 FIT IN THE HIGHEST RESOLUTION BIN.
     REMARK 3
                                                               20
                  TOTAL NUMBER OF BINS USED
     REMARK
                                                             2.601
                  BIN RESOLUTION RANGE HIGH
     REMARK
                  BIN RESOLUTION RANGE LOW
                                                             2.668
     REMARK
              3 REFLECTION IN BIN (WORKING SET) :
3 BIN R VALUE (WORKING SET) :
                                                             2799.
35
     REMARK
                                                              0.282
              3. BIN R VALUE
     REMARK
                  BIN FREE R VALUE SET COUNT
                                                              145
     REMARK 3
                                                              0.403
                   BIN FREE R VALUE
     REMARK
     REMARK
     REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
40
                                         : 9531
             3
                  ALL ATOMS
      REMARK
     REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (ARMARK 3 MEAN B VALUE (OVERALL, ARMARK 3 OVERALL ANISOTROPIC B VALUE.
               3 B VALUES.
3 FROM WILSON PLOT (A**2) : NULL
3 MEAN B VALUE (OVERALL, A**2) : 50.041
      REMARK 3 B11 (A**2): -4.02
                                    -0.68
                  B22 (A**2) :
      REMARK 3
      REMARK 3 B33 (A**2): 4.60
REMARK 3 B12 (A**2): 0.00
                   B13 (A**2) : -0.24
B23 (A**2) : 0.00
      REMARK 3
      REMARK 3
      REMARK 3
      REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
                   ESU BASED ON R VALUE
      REMARK 3
 55
                                                                      (A): 0.408
      REMARK 3
                   ESU BASED ON FREE R VALUE
                                                                            0.512
                   ESU BASED ON MAXIMUM LIKELIHOOD
                                                                      (A):
      REMARK
               3.
                   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 23.746
      REMARK
      REMARK
              3 CORRELATION COEFFICIENTS.
 60
      REMARK
```

PCT/GB02/03461

```
CORRELATION COEFFICIENT FO-FC
    REMARK . 3
                 CORRELATION COEFFICIENT FO-FC FREE:
            · 3
    REMARK
    REMARK
             3
                                                                        WEIGHT
                                                        COUNT
                                                                 RMS
                 RMS DEVIATIONS FROM IDEAL VALUES
    REMARK
                                                    (A): 9582; 0.022; 0.021
                 BOND LENGTHS REFINED ATOMS
    REMARK
                                                    (A): 8445; 0.001; 0.020
                 BOND LENGTHS OTHERS
              3
10
     REMARK
                                              (DEGREES): 13011 ; 2.356 ; 1.945
                  BOND ANGLES REFINED ATOMS
     REMARK
              3
                                              (DEGREES): 19641; 0.973; 3.000
                  BOND ANGLES OTHERS
     REMARK
              3
                                              (DEGREES): 1173; 6.207; 3.000
                  TORSION ANGLES, PERIOD 1
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              3
                                              (DEGREES): 1607;21.762;15.000
                  TORSION ANGLES, PERIOD 3
     REMARK
                                                 (A**3): 1422; 0.121; 0.200
                  CHIRAL-CENTER RESTRAINTS
   REMARK
15
                                                   (A): 10704; 0.003; 0.020
                  GENERAL PLANES REFINED ATOMS
     REMARK
                                                    (A): 2010; 0.001; 0.020
                  GENERAL PLANES OTHERS
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              3
                  NON-BONDED CONTACTS REFINED ATOMS (A): 2679; 0.339; 0.300
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              3
                                                    (A): 9125; 0.264; 0.300
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              3
     REMARK
                                                           3; 0.093; 0.500
                                                    (A):
                  NON-BONDED TORSION OTHERS
              3
20
     REMARK
                                                           834 ; 0.226 ; 0.500
                  H-BOND (X...Y) REFINED ATOMS
                                                    (A):
     REMARK
                                                           35 ; 0.161 ; 0.500
                  H-BOND (X...Y) OTHERS
                                                    (A):
     REMARK
                                                            20 ; 0.299 ; 0.300
                                                    (A):
                  SYMMETRY VDW REFINED ATOMS
     REMARK
                                                    (A):
                                                            62 ; 0.395 ; 0.300
                  SYMMETRY VDW OTHERS
     REMARK
              3
                                                            10 ; 0.351 ; 0.500
                  SYMMETRY H-BOND REFINED ATOMS
                                                    (A):
     REMARK
                                                             2; 0.229; 0.500
                  SYMMETRY H-BOND OTHERS
                                                    (A):
     REMARK
     REMARK
                 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                          COUNT
     REMARK
                  MAIN-CHAIN BOND REFINED ATOMS (A**2): 5889; 3.453; 5.000
     REMARK
                  MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 9501; 5.002; 6.000
30
     REMARK
                                                          3693 ; 4.504 ; 6.000
                  SIDE-CHAIN BOND REFINED ATOMS (A**2):
     REMARK
                                                          3510 ; 6.644 ; 7.500
                  SIDE-CHAIN ANGLE REFINED ATOMS (A**2):
     REMARK
     REMARK
                 NCS RESTRAINTS STATISTICS
     REMARK
                  NUMBER OF NCS GROUPS : NULL
35
     REMARK
               3
     REMARK
               3
     REMARK
                 TLS DETAILS
     REMARK
              3
                  NUMBER OF TLS GROUPS : NULL
     REMARK
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     REMARK
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      REMARK
                   METHOD USED : BABINET MODEL WITH MASK
      REMARK
                   PARAMETERS FOR MASK CALCULATION
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      REMARK
                   VDW PROBE RADIUS : 1.40
 45
      REMARK
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                                      :
                                         0.80
                   ION PROBE RADIUS
      REMARK
               3
                   SHRINKAGE RADIUS
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      REMARK
                 OTHER REFINEMENT REMARKS:
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      CISPEP
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                               PRO A 129
               2 ARG'A 128
      CISPEP
                                                             0.00
               3 GLY A 372
                               PRO A 373
      CISPEP
                               CYS A
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               1 CYS A 155
 55
      SSBOND
                               CYS A
                                      382
      SSBOND.
               2 CYS A 217
               3 CYS A 269
                               CYS A
                                      319
      SSBOND
                                                             0.00
               4 SER B
                       22
                               PRO B
                                       23
      CISPEP
                                                             0.00
                               PRO B
                                      129
      CISPEP
               5 ARG B 128
                                                             0.00
                               PRO B
                                      373
               6 GLY B
                        372
      CISPEP
 60
                               CYS B
                                      359
               4 CYS B
                        155
      SSBOND
```

```
217
                               CYS B
                                      382
5
     SSBOND
              5 CYS B
                               CYS B
                                       319
              6 CYS B
                        269
     SSBOND
                         22
                               PRO C
                                       . 23
                                                               0.00
              7 SER C
     CISPEP
                                                               0.00
     CISPEP
              8 ARG C
                        128
                               PRO C
                                       129
                                                               0.00
                               PRO C
                                       373
              9 GLY C
                        372
     CISPEP
              7 CYS C
                        155
                               CYS C
                                       359
10
     SSBOND
              8 CYS C
                        217
                               CYS C
                                       382
     SSBOND
                               CYS C
                                      319
     SSBOND
              9 CYS C
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                                                        0:00000
                 0.000000
                            0.000000
                                      0.016294
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                              -2
               3 CA
                      SER A
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                                                                                       C
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                                                                                       С
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                              -1
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              33
                  0
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                                0
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35
              36
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                                                                                       C
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                  CB
                                0
                                                                                       C
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                                                        16.565
                                                                 1.00 59.81
                  CG1 VAL A
     MOTA
              40
                                O
                  CG2 VAL A
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                                                                 1.00 54.45
                                                                                       С
              44
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                                                                 1.00 47.63
                                                                                       С
     MOTA
              48
                  С
                       VAL A
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                                                                                       O
40
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              50
                  N
                       GLU A
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              52
                  CA
                       GLU A
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                                       24.489 -19.994
                                                        16.474
                                                                 1.00 46.47
              54
                   CB
                       GLU A
                                1
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                                       23.893 -20.218
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              57
                   CG
                       GLU A
                                1
                                                        15.070
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                                                                                       C
45
               60
                   CD
                       GLU A
                                1
                                       24.627 -21.224
                                                        14.257
                                                                 1.00 36.90
     ATOM
                                                                                       0
                                                                 1.00 29.13
                   OE1 GLU A
                                       23.964 -21.926
                                                        13.487
     MOTA
               61
                                1
                                                                                       0
                                                                 1.00 44.61
               62
                   OE2 GLU A
                                1
                                       25.868 -21.304
                                                        14.382
     MOTA
                       GLU A
                                       23.573 -17.933
                                                        17.273.
                                                                 1.00 44.07
                                                                                       Ċ
     ATOM
               63
                   С
                                1
                                       23.950 -17.227
                                                                                       0
     ATOM
               64
                   0
                       GLU A
                                1
                                                        18.185
                                                                 1.00 47.47
                       MET A
                                      23.211 -17.471
                                                        16.087
50
                                2
                                                                 1.00 48.56
     ATOM
               65
                   N.
                                       23.536 -16.135
                       MET A
                                                        15.628
                                                                 1.00 44.26
               67
                   CA
                                2
     MOTA
                                                                                       C
                   CB
                       MET A
                                       23.886 -16.271
                                                        14.156
                                                                1.00 46.78
               69
                                2
     ATOM
                                      24.968 -17.287
                                                                                       С
                                                        13.979
                                                                 1.00 46.07
               72
                   CG
                       MET A
                                2
     MOTA
                                     25.968 -17.107
               75
                   SD
                       MET A
                                                        12.614
                                                                 1.00 44.85
                                2
     MOTA
                                                        11.580
                                                                                       С
55
              76
                   CE
                       MET A
                                2
                                       25.329 -18.379
                                                                 1.00 47.63
     MOTA
                                                                                       C
               80
                   С
                       MET A
                                2
                                       22.441 -15.143
                                                        15.782
                                                                 1.00 44.93
     MOTA
                                                                                       0
                       MET A
                                       22.694 -13.949
                                                        15.928
                                                                 1.00 44.66
     ATOM
               81
                   0
                                2
                       VAL A
                                       21.213 -15.640
                                                        15.739
                                                                 1.00 44.93
                                                                                       N
               82
                   N
                                3
     MOTA
               84
                   CA
                       VAL A
                                       20.054 -14.792
                                                        15.864
                                                                 1.00 42.74
                                                                                       С
                                3
     ATOM
                                       18.787 -15.658
                                                        15.886
60
     ATOM
               86
                   CB
                       VAL A
                                3
                                                                 1.00 41.67
                   CG1 VAL A
                                       17.725 -15.033
                                                        16.713
                                                                 1.00 37.90
     ATOM
               88
                                3
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•						•							
5	ATOM	. 92	CG2	VAL	A	3		18.319	-15.879	14.506	1.00 37.99	_	С
	ATOM	96	C	VAL	Α	3		20.178	-14.009	17.153	1.00 43.63		C
	MOTA	97	0	VAL	Α	3		20.474	-14.592	18.164	1.00 38.26	•	O
	ATOM	98	N	ASP	A.	4		19.953	-12.696	17.100	1.00 45.42		N
	ATOM	100	CA	ASP	Α	4		20.026	-11.823	18.267	1.00 45.76		С
10	ATOM	102	CB	ASP	Α	4		19.330	-12.445	19.482	1.00 53.20		С
	ATOM	105	CG	ASP	A	4		17.803	-12.638	19.299	1.00 65.48		С
	ATOM	106		ASP		4			-13.367	20.153	1.00 74.58		Ο.
	MOTA	107		ASP		4			-12.144	18.367	1.00 62.82	•	0
	ATOM	108	C	ASP		4	-	21.417	-11.521	18.742	1.00 45.27		С
15	ATOM	109	ò	ASP		4			-11.253	19.923	1.00 50.54		0
13	ATOM	110	N	ASN		5			-11.539	17.888	1.00 41.26		N
	ATOM	112	CA	ASN		5			-11.339	18.387	1.00 35.44	•	С
	ATOM	114	СВ	ASN		. 5	•		-12.331	17.728	1.00 37.18	•	С
•	ATOM	117	CG	ASN		.5			-12.137	16.262	1.00 39.34		С
20	ATOM	118		ASN		5			-11.544	15.736	1.00 38.77		0
20	ATOM	119.		ASN		5			-12.618	15.586	1.00 35.75		N
	ATOM	122	C	ASN		5		24.387	-9.939	18.228	1.00 38.11		C
	ATOM	123	Ö	ASN		5		25.585	-9.733		1.00 37.36	*	Ö
			N	LEU		: 6	•	23.549	-8.980	17.833	1.00 38.41		N
25	ATOM	124		LEU		6		23.939	-7.572	17.679	1.00 33.19		Ċ
25	ATOM	126	CA	LEU		6		23.468	-7.098	16.340	1.00 26.93		Ċ.
	ATOM	128	CB					24.086	-7.474	15.007	1.00 27.79		Ċ
	ATOM	131	CG	LEU		6.			-6.361	14.059	1.00 27.73		č
	MOTA	133		LEU		6		23.717		14.039	1.00 27.07	•	c
20	ATOM	137		LEU		6		25.567	-7.678		1.00 22.82		Ċ
30	MOTA	141	C	LEU		6.		23.293	-6.664	18.756			Ö
	ATOM	142	0	LEU		6		22.262	-7.002	19.284	1.00 46.36		
	ATOM	143	N	ARG		. 7		23.875	-5.513	19.075	1.00 41.26		N C
:	MOTA	145	CA	ARG		7		23.290	-4.554	20.038	1.00 40.38		
	ATOM	147	CB	ARG		7		23.833	-4.740	21.451	1.00 44.61		C
35	MOTA	150		ARG		7		23.137	-5.889	22.209	1.00 57.60		C
	MOTA	153	CD	ARG		7		23.680	-6.233	23.630	1.00 65.11		
	ATOM	156	NE	ARG		7		25.141	-6.399	23.667	1.00 76.98		N
	ATOM	158	CZ	ARG		7		25.947	-6.088	24.706	1.00 82.43		C
	ATOM	159		ARG		7		25.468	-5.589	25.845	1.00 83.89		N
40	ATOM	162		ARG		7		27.256	-6.284	24.603	1.00 82.28		N
	MOTA	165	С	ARG		7		23.627	-3.196	19.506	1.00 37.09		C
	ATOM	166	0	ARG		7		24.329	-3.119	18.506	1.00 39.77		0
	MOTA	167	N	GLY		8		23.139	-2.136	20.139	1.00 41.94	•	N
	MOTA	169	CA	GLY	A	. 8		23.316	-0.770	19.642	1.00 46.85		C
45	ATOM	172	C	GLY		8.		22.093		18.994	1.00 53.78		С
	MOTA	173	0	GLY	Α	8		20.926	-0.485	19.254	1.00 49.83		0
	MOTA	174	N	LYS		9		22.345	0.968	18.169	1.00 56.06		N
	MOTA	176	CA	LYS	A	9		21.272		17.372	1.00 58.92		С
	ATOM	178	CB	LYS	Α	. 9		20.312	2.324	18.314	1.00 65.60		С
50	ATOM	181	CG	LYS	A	9		20.817	3.673	18.821	1.00 71.58		C
	ATOM	184	CD	LYS	A	. 9		19.785	. 4.339	19.712.			С
	ATOM	187	CE.	LYS	Α	9		20.460	5.364	20.645	1.00 81.30	. *	С
	ATOM	190	· NZ	LYS	Α	9		19.689	5.694	21.898	1.00 79.59		N
	ATOM	194	C .	LYS		. 9		21.662	2.497	16.157	1.00 57.10		, c
55	ATOM	195	Ö	LYS		. 9		22.801		15.996	1.00 53.27		, 0
	MOTA	196	N	SER		10	: `	20.691		15.312	1.00 58.39		N
	ATOM	198	CA	SER		10		21.022		14.153			С
	ATOM	200	СВ	SER		10		19.791		13.417		•	С
	ATOM	203	OG	SER		10		18.789		14.345	1.00 73.85		0
60	ATOM	205	c	SER		10		21.724			1.00 61.22		С
00	ATOM	206	Ö	SER		10		22.617		13.956	1.00 64.24		o
	MION	200	9	CUIN		_~			5, 101				

ATOM 209 CA GLY A 11 21.807 6.519 16.499 1 ATOM 212 C GLY A 11 23.308 6.455 16.511 ATOM 213 0 GLY A 11 23.308 6.457 17.7052 1 ATOM 214 N GLN A 12 23.864 5.357 17.052 1 ATOM 216 CA GLN A 12 25.656 5.405 18.653 1 ATOM 216 CA GLN A 12 25.656 5.405 18.653 1 ATOM 221 CG GLN A 12 25.656 5.405 18.653 1 ATOM 221 CG GLN A 12 25.254 6.733 19.190 1 ATOM 222 CG GLN A 12 25.455 6.803 20.686 1 ATOM 225 OE1 GLN A 12 25.455 6.803 20.686 1 ATOM 226 NE2 GLN A 12 25.455 6.803 20.686 1 ATOM 226 NE2 GLN A 12 25.959 3.922 16.774 1 ATOM 229 C GLN A 12 25.959 3.922 16.774 1 ATOM 230 O GLN A 12 25.939 3.922 16.774 1 ATOM 231 N GLY A 13 25.264 3.200 15.897 ATOM 233 CA GLY A 13 25.260 0.639 16.051 ATOM 233 CA GLY A 13 25.260 0.639 16.051 ATOM 237 O GLY A 13 25.250 0.639 16.051 ATOM 238 N TYR A 14 25.256 -0.415 15.219 ATOM 240 CA TYR A 14 25.256 -0.415 15.219 ATOM 240 CA TYR A 14 25.256 -0.415 15.219 ATOM 240 CA TYR A 14 22.871 -1.882 14.569 ATOM 246 CGL TYR A 14 22.871 -1.882 14.579 ATOM 246 CGL TYR A 14 22.871 -1.882 14.579 ATOM 247 CGL TYR A 14 22.871 -1.882 14.579 ATOM 248 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CA TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 240 CGL TYR A 14 22.871 -1.882 14.579 ATOM 250 CC TYR A 14 20.659 -2.045 15.246 ATOM 250 CC TYR A 14 20.659 -2.045 15.246 ATOM 250 CC TYR A 14 20.659 -2.045 15.246 ATOM 250 CC TYR A 15 20.411 -0.876 14.617 ATOM 260 CGL TYR A 15 20.600 -3.917 16.966 ATOM 250 CC TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 ATOM 260 CGL TYR A 15 20.900 -2.934 19.303 11.6.316 ATOM 290 CGL TYR A 15 20.900 -2.934 19.3																
ATOM 209 CA GLY A 11 21.807 6.519 16.499 17.404 11.4 21.308 6.455 16.511 1 ATOM 213 O GLY A 11 23.308 6.455 16.511 1 ATOM 214 N GLN A 12 23.864 5.357 17.050 18.600 19.600	5	ATOM	207	N	GLY	Α	11		21.279	5.370	15.818	1.00	60.57			N
ATOM 213 C GLY A 11 23.308 6.455 16.511 3 ATOM 214 N GLN A 12 23.952 7.390 16.020 17.052 1 10 ATOM 216 CA GLN A 12 23.864 5.357 17.052 1 10 ATOM 216 CA GLN A 12 25.513 5.236 17.206 1 ATOM 218 CB GLN A 12 25.555 5.405 18.653 19.190 1 ATOM 221 CG GLN A 12 25.555 6.5405 18.653 19.190 1 ATOM 224 CD GLN A 12 25.555 6.803 20.686 1 ATOM 225 CEI GLN A 12 25.455 6.803 20.686 1 ATOM 225 CEI GLN A 12 25.155 5.827 21.393 19.190 1 ATOM 225 CEI GLN A 12 25.950 7.941 21.174 1 ATOM 229 C GLN A 12 25.950 7.941 21.174 1 ATOM 220 C GLN A 12 25.939 3.922 16.774 1 ATOM 230 C GLN A 12 27.027 3.567 17.245 ATOM 231 N GLY A 13 25.264 3.200 15.897 ATOM 233 CA GLY A 13 25.264 3.200 15.897 ATOM 237 C GLY A 13 25.264 3.200 15.897 ATOM 237 C GLY A 13 25.265 0.639 16.051 ATOM 237 C GLY A 13 25.266 0.415 15.219 ATOM 238 C GLY A 13 25.250 0.639 16.051 ATOM 238 N TYR A 14 25.256 0.415 15.219 ATOM 240 CA TYR A 14 25.256 0.415 15.219 ATOM 240 CA TYR A 14 25.256 0.415 15.219 ATOM 245 CG TYR A 14 25.256 0.415 15.219 ATOM 246 CDI TYR A 14 22.871 -1.882 14.579 ATOM 248 CEI TYR A 14 22.871 -1.882 14.579 ATOM 250 CZ TYR A 15 26.590 -2.045 14.603 ATOM 250 CZ TYR A 15 26.590 -2.045 14.603 ATOM 250 CZ TYR A 15 26.590 -2.045 14.603 ATOM 250 CZ TYR A 15 27.922 -1.787 16.965					GLY .	A	11		21.807	6.519	16.499	1.00	49.93			C
ATOM 213 O GLY A 11 23,952 7,390 16,020 1 ATOM ATOM 214 N GLN A 12 23,864 5,357 17,052 17,052 18 ATOM 218 CB GLN A 12 25,313 5,236 17,206 1 ATOM 218 CB GLN A 12 25,656 5,405 18,653 1 ATOM 221 CG GLN A 12 25,254 6,733 19,190 1 ATOM 221 CG GLN A 12 25,254 6,733 19,190 1 ATOM 225 OE1 GLN A 12 25,254 6,733 19,190 1 ATOM 225 OE1 GLN A 12 25,256 6,733 19,190 1 ATOM 225 OE1 GLN A 12 25,956 7,941 21,174 1 ATOM 229 C GLN A 12 25,960 7,941 21,174 1 ATOM 230 N GLN A 12 25,960 7,941 21,174 1 ATOM 231 N GLY A 13 25,264 3,200 15,897 ATOM 231 N GLY A 13 25,264 3,200 15,897 ATOM 231 N GLY A 13 25,264 3,200 15,897 ATOM 231 N GLY A 13 25,260 0,639 16,051 ATOM 236 C GLY A 13 25,763 1,941 15,424 1 ATOM 237 N GLY A 13 25,250 0,639 16,051 ATOM 237 N GLY A 13 25,250 0,639 16,051 ATOM 240 CA TYR A 14 25,070 -1.777 15,613 ATOM 240 CA TYR A 14 25,070 -1.777 15,613 ATOM 240 CA TYR A 14 22,871 -1.882 14,579 ATOM 246 CD1 TYR A 14 22,871 -1.882 14,579 ATOM 248 CE1 TYR A 14 22,871 -1.882 14,579 ATOM 248 CE1 TYR A 14 22,871 -1.882 14,579 ATOM 248 CE1 TYR A 14 22,871 -1.882 14,579 ATOM 250 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 14 20,411 -0.876 14,617 ATOM 257 CZ TYR A 15 27,905 -3.917 16,096 ATOM 258 CZ TYR A 15 28,659 -2.945 17,686 ATOM 257 CZ TYR A 15 27,905 -3.917 16,096 ATOM 258 CZ TYR A 15 27,905 -3.917 16,096 ATOM 266 CB TYR A 15 27,905 -3.917 16,096 ATOM 266 CB TYR A 15 27,905 -3.917 16,096 ATOM 270 CD TYR A 15 27,905 -3.917 16,096 ATOM 270 CD TYR A 15 27,905 -3.917 16,095 ATOM 270 CD TYR A 15 27,905 -3.917 16,095 ATOM 270 CD TYR							11		23.308	6.455	16.511	1.00				С
ATOM					GLY .	Α	11		23.952	7.390	16.020	1.00				0
10 ATM									23.864	5.357	17.052	1.00	51.87			N
ATOM 218 CB GLN A 12 25.656 5.405 18.653 1 ATOM 221 CG GLN A 12 25.254 6.733 19.190 1 ATOM 221 CD GLN A 12 25.455 6.803 20.686 1 ATOM 225 OE1 GLN A 12 25.455 6.803 20.686 1 ATOM 226 NE2 GLN A 12 25.155 5.827 21.393 1 ATOM 226 NE2 GLN A 12 25.959 7.941 21.174 1 ATOM 229 C GLN A 12 25.939 3.922 16.774 1 ATOM 230 O GLN A 12 27.027 3.567 17.245 ATOM 231 N GLY A 13 25.264 3.200 15.897 ATOM 231 N GLY A 13 25.264 3.200 15.897 ATOM 233 CA GLY A 13 25.264 3.200 15.897 ATOM 237 O GLY A 13 25.250 0.639 16.051 ATOM 237 O GLY A 13 25.250 0.639 16.051 ATOM 240 CA TYR A 14 25.070 -1.777 15.616 ATOM 240 CA TYR A 14 25.070 -1.777 15.616 ATOM 240 CB TYR A 14 24.228 -2.432 14.566 ATOM 245 CB TYR A 14 22.592 -0.703 13.951 ATOM 246 CD1 TYR A 14 22.592 -0.703 13.951 ATOM 248 CE1 TYR A 14 22.592 -0.703 13.951 ATOM 250 CZ TYR A 14 20.411 -0.876 14.638 ATOM 255 CD2 TYR A 14 20.411 -0.876 14.637 ATOM 255 CD2 TYR A 14 20.451 -0.405 14.638 ATOM 255 CD2 TYR A 14 20.451 -0.405 14.638 ATOM 258 O TYR A 15 26.610 -3.291 16.734 ATOM 258 O TYR A 15 26.610 -3.291 16.734 ATOM 258 O TYR A 15 26.659 -2.045 15.246 ATOM 259 N TYR A 15 26.610 -3.291 16.734 ATOM 259 N TYR A 15 26.610 -3.291 16.734 ATOM 266 CG TYR A 15 27.905 -3.917 16.966 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.885 ATOM 267 CD1 TYR A 15 27.661 -4.030 21.388 4CB TYR A 15 27.664 -2.892 21.88	10								25.313	5.236	17.206	1.00	51.01			С
ATOM 221 CG GIN A 12 25.254 6.733 19.190 1 ATOM 224 CD GIN A 12 25.455 6.803 20.686 1 ATOM 225 OEI GIN A 12 25.155 5.827 21.393 3 15 ATOM 226 NE2 GIN A 12 25.939 3.922 16.774 1 ATOM 229 C GIN A 12 25.939 3.922 16.774 1 ATOM 230 O GIN A 12 27.027 3.567 17.245 1 ATOM 231 N GIY A 13 25.264 3.200 15.897 17.245 1 ATOM 233 CA GIY A 13 25.264 3.200 15.897 17.245 1 ATOM 233 CA GIY A 13 25.250 0.639 16.051 1 ATOM 237 O GIY A 13 25.250 0.639 16.051 1 ATOM 238 N TYR A 14 25.250 0.639 16.051 1 ATOM 240 CA TYR A 14 25.250 0.639 16.051 1 ATOM 240 CA TYR A 14 25.250 0.639 16.051 1 ATOM 240 CA TYR A 14 25.250 0.639 16.051 1 ATOM 245 CG TYR A 14 25.250 0.71777 15.613 1 ATOM 246 CD1 TYR A 14 22.887 1 -1.882 14.576 1 ATOM 248 CEI TYR A 14 22.887 1 -1.882 14.579 1 ATOM 250 CZ TYR A 14 20.411 0.876 14.617 1 ATOM 251 OH TYR A 14 20.411 0.876 14.638 1 ATOM 255 CD2 TYR A 14 20.659 -2.045 15.246 1 ATOM 255 CD2 TYR A 14 20.659 -2.045 15.246 1 ATOM 258 O TYR A 14 26.388 -2.532 15.264 1 ATOM 258 O TYR A 14 26.388 -2.532 15.264 1 ATOM 259 N TYR A 15 26.610 -3.291 16.734 1 ATOM 260 CG TYR A 15 27.905 -3.917 16.966 1 ATOM 261 CA TYR A 15 27.905 -3.917 16.966 1 ATOM 267 CD1 TYR A 15 28.655 -2.978 17.805 1 ATOM 268 CG TYR A 15 28.655 -2.978 17.805 1 ATOM 269 CEI TYR A 15 27.905 -3.917 16.966 1 ATOM 271 CZ TYR A 15 27.905 -3.917 16.966 1 ATOM 272 OH TYR A 15 28.655 -2.978 17.805 1 ATOM 274 CEZ TYR A 15 27.905 -3.917 16.966 1 ATOM 275 C TYR A 15 27.905 -3.917 17.605 1 ATOM 276 CD2 TYR A 15 27.905 -3.917 17.605 1 ATOM 279 O TYR A 15 27.925 -7.544 17.308 17.30	10										18.653	1.00	50.53			С
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ATOM 278 C TYR A 15 27.828 -5.307 17.605 45 ATOM 279 O TYR A 15 26.901 -5.608 18.296 ATOM 280 N VAL A 16 28.832 -6.148 17.398 ATOM 282 CA VAL A 16 28.763 -7.554 17.781 ATOM 284 CB VAL A 16 28.826 -8.444 16.556 ATOM 286 CG1 VAL A 16 30.280 -8.691 16.154 50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 30.339 -10.181 21.407 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 30.339 -11.380 23.676 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538		ATOM	274	CE2	TYR	Α	15		27.023	-1.757			41.62		-	С
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ATOM 280 N VAL A 16 28.832 -6.148 17.398 ATOM 282 CA VAL A 16 28.763 -7.554 17.781 ATOM 284 CB VAL A 16 28.826 -8.444 16.556 ATOM 286 CG1 VAL A 16 30.280 -8.691 16.154 50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 30.339 -10.181 21.407 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 30.339 -11.380 23.676 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538	45		279	O.	TYR	A.	15		26.901	-5.608	18.296		33.91			0
ATOM 282 CA VAL A 16 28.763 -7.554 17.781 ATOM 284 CB VAL A 16 28.826 -8.444 16.556 ATOM 286 CG1 VAL A 16 30.280 -8.691 16.154 50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 30.339 -10.181 21.407 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 30.339 -11.380 23.676 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538			280	N·	VAL	A	16		28.832	-6.148	17.398	1.00	38.82			N
ATOM 284 CB VAL A 16 28.826 -8.444 16.556 ATOM 286 CG1 VAL A 16 30.280 -8.691 16.154 50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 30.339 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 30.339 -11.380 23.676 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538			282	CA	VAL	Α	16		28.763	-7.554	17.781	1.00	36.77			С
ATOM 286 CG1 VAL A 16 30.280 -8.691 16.154 50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 30.339 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538				CB			16		28.826	-8.444	16.556	1.00	41.62			С
50 ATOM 290 CG2 VAL A 16 28.212 -9.788 16.804 ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538									30.280	-8.691	16.154	1.00	41.85			С
ATOM 294 C VAL A 16 29.993 -7.861 18.579 ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538	50									-9.788		1.00	46.15			C
ATOM 295 O VAL A 16 30.995 -7.188 18.388 ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538	50											1.00	37.30			C
ATOM 296 N GLU A 17 29.898 -8.861 19.461 ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538								•					37.00			Q .,
ATOM 298 CA GLU A 17 30.974 -9.315 20.309 55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538									•				32.42			Ņ
55 ATOM 300 CB GLU A 17 30.339 -10.181 21.407 ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538													37.70		•	Ċ
ATOM 303 CG GLU A 17 31.155 -10.529 22.669 ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538	55												41.03			С
ATOM 306 CD GLU A 17 30.339 -11.380 23.676 ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538	در												41.42			Č
ATOM 307 OE1 GLU A 17 29.191 -10.947 24.041 ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538									•				53.52			C
ATOM 308 OE2 GLU A 17 30.807 -12.484 24.114 60 ATOM 309 C GLU A 17 32.000 -10.162 19.538								•					62.24			ŏ
60 ATOM 309 C GLU A 17 32.000 -10.162 19.538													47.86	•		. 0
	C 0												39.46			c
ATOM 310 O GLU A 1/ 31.63/ ~11.032 18./96	60															o
		ATOM	310	O	GLU	A	17		31.03/	-11.032	10.130	1.00	39.58			•

						• •	
5	ATOM	311	N	MET A	18	33.292 -9.925 19.711 1.00 44.75	N
_	ATOM	313	CA	MET A	18	34.301 -10.791 19.082 1.00 41.54	C
	MOTA	315	CB	MET A	18	34.838 -10.160 17.802 1.00 41.81	С
	ATOM	318	CG	MET A	18	33.836 -9.447 16.939 1.00 41.86	C
	ATOM	321	SD	MET A	18	34.600 -8.833 15.425 1.00 50.01	s
10.	ATOM	322	CE	MET A	18	35.054 -10.282 14.687 1.00 45.99	С
	ATOM	326	С	MET A	18	35.466 -10.864 20.038 1.00 43.74	С
	ATOM	327	0	MET A	18	35.596 -10.003 20.877 1.00 49.03	0
	ATOM	328	N	THR A	19	36.325 -11.868 19.937 1.00 45.52	N
	ATOM	330	CA	THR A	19	37.572 -11.813 20.698 1.00 45.53	С
15	MOTA	332	CB	THR A	19	37.747 -13.023 21.572 1.00 45.33	С
	ATOM	334	OG1	THR A	19	38.226 -14.108 20.759 1.00 50.86	0
	MOTA	336	CG2	THR A	19	36.463 -13.451 22.142 1.00 40.03	С
	ATOM	340	С	THR A	19	38.763 -11.893 19.814 1.00 45.19	С
•	ATOM	341	0	THR A	19	38.693 -12.560 18.785 1.00 47.81	0
20 .	ATOM	342	N	VAL A	20	39.865 -11.267 20.243 1.00 46.54	N
	ATOM	344	CA	VAL A	20	41.181 -11.385 19.556 1.00 46.08	С
	ATOM	346	CB.	VAL A	20	41.657 -10.076 19.031 1.00 44.11	С
	ATOM	348	CG1	VAL A	20	40.734 -9.589 17.998 1.00 51.93	С
	ATOM	352	CG2	VAL A	20	41.687 -9.058 20.110 1.00 51.31	С
25	ATOM	356	С	VAL A	20	42.286 -11.858 20.490 1.00 48.60	С
	ATOM	357	0	VAL A	20	42.242 -11.643 21.715 1.00 49.22	0
	ATOM	358	N	GLY A	21	43.293 -12.505 19.944 1.00 49.38	N
	ATOM	360	CA	GLY A	. 21	44.406 -12.881 20.791 1.00 51.59	C
	ATOM	363	С	GLY A	21	44.282 -14.129 21.652 1.00 51.96	С
30	ATOM	364	0	GLY A	21	43.216 -14.659 21.926 1.00 48.04	0
	ATOM	365	N	SER A	22	45.430 -14.604 22.087 1.00 51.50	N
	ATOM	367	CA	SER A	22	45.462 -15.754 22.916 1.00 54.86	C
	MOTA	369	CB	SER A		46.238 -16.846 22.176 1.00 58.86	.C
	MOTA	. 372	· OG	SER A		45.861 -16.909 20.794 1.00 60.35	0
35	MOTA	374	Ç	SER A		46.156 -15.336 24.203 1.00 54.80	С
•	MOTA	375	Ò	SER A		47.217 -14.720 24.127 1.00 53.24	.0
	MOTA	376	N	PRO A		45.551 -15.566 25.378 1.00 54.99	N
	MOTA	377	CA	PRO A		44.141 -15.954 25.547 1.00 56.89	С
	ATOM	. 379	CB	PRO A		43.945 -15.868 27.056 1.00 54.92	C
40	ATOM	382	CG	PRO A		45.075 -15.007 27.510 1.00 52.28	C
	MOTA	385	CD	PRO A		46.218 -15.491 26.680 1.00 53.62	C C
	MOTA	388	С	PRO A		43.244 -14.889 24.943 1.00 56.89	0
	MOTA	389	0	PRO A		43.808 -13.858 24.604 1.00 57.85	N
	MOTA	390	N	PRO A		41.931 -15.125 24.840 1.00 56.03	C
45	ATOM	391		PRO A		40.963 -14.220 24.217 1.00 52.69	c
	MOTA	393	CB	PRO A		39.667 -15.023 24.276 1.00 52.70 40.058 -16.369 24.440 1.00 55.89	C
•	ATOM	396	CG	PRO A		•	c
	MOTA	399.		PRO A			c
	ATOM	402		PRO A		40.697 -12.963 24.971 1.00 52.11	Ö
50°	MOTA	403	0	PRO A		40.598 -13.028 26.170 1.00 56.31 40.558 -11.856 24.261 1.00 53.37	N
	ATOM	. 404	N	GLN A			C ·
:	ATOM	406	CA	GLN A			Ċ.
	MOTA	408	. CB.	GLN A			. c
	ATOM	411	CG	GLN A			· c
55	MOTA	414	CD	GLN A			ō
	ATOM	415	OE1				N
	MOTA	416		GLN A			C
	ATOM	419	C	GLN A			o
-	ATOM	420	0	GLN A			N
60	MOTA	421	N	THR A			C
	MOTA	423	CA	THR A	A 26	36.604 -9.597 24.436 1.00 50.69	C

•	7 MOM	405	СВ	THR	Δ	26		35.614	-9.763	25.531	1.00	49.93		C	
5	MOTA.	425		THR		26		35.404	-11.164	25.799	1.00	53.75		C	
	MOTA	427		THR		26		34.308	-9.246	25.060	1.00	46.30		C	
	ATOM	429	CGZ	THR		26		36.575		24.003	1.00	51.52		(7
	ATOM	433		THR		26		37.078	-7.284	24.696		59.94		()
10	ATOM	434	0	LEU		27		35.982	-7.856	22.858		49.68		ì	
10	MOTA	435	N	LEU		27		35.858	-6.476	22.412		39.53			2
	MOTA	437	CA	PÉO		27		37.066	-6.094	21.592		42.69			2
	MOTA	439	CB CG	LEU		27		38.456	-5.850	22.241		44.73			3
	MOTA	442		LEU		27		39.404	-5.301	21.192	1.00	42.23			С
	MOTA	444		LEU		27		38.418	-4.865	23.382	1.00	44.45			C i
15	ATOM	448	CDZ	LEU		27		34.615	-6.390	21.574	1.00	40.04			С
	ATOM	452		LEU		27		34.313	-7.319	20.821	1.00	40.69		. (0
	MOTA	453	O N	ASN.		28		33.859	-5.305	21.704	1.00	43.27			N
	ATOM	454		ASN		28		32.654	-5.129	20.873	1.00	43.26			С
20	MOTA	456	CA	ASN		28		31.509	-4.465	21.654	1.00	45.19			С
20	ATOM	458	CB CG	ASN		28		30.830	-5.417	22.672	1.00	44.78		1	C
	MOTA	461		ASN		28		30.936	-5.234	23.888		47.19			0
	MOTA	462		ASN		28		30.123	-6.411	22.174		42.58			N
	MOTA	463	C	ASN		28		33.018	-4.308	19.633	1.00	45.28			С
25	ATOM	466		ASN		28		33.476	-3.172	19.775		46.40	٠.		0
25	MOTA	467	0 N	ILE		29		32.795	-4.911	18.450	1.00	46.88			N
	ATOM	468	N CA	ILE		29		33.115	-4.400	17.094	1.00	44.20			C
	MOTA	470	CB	ILE		29		33.690	-5.561	16.303		43.47			С
	MOTA	474		ILE		29		34.737	-6.291	17.121	1.00	43.10			С
20	MOTA	477		ILE		29		35.870	-5.421	17.574		44.94	•		С
30	MOTA	481		ILE		29		34.248	-5.079	14.973		46.96			С
	ATOM ATOM	485	Ç	ILE		29		31.942	-3.874			41.20			C
	ATOM	486	ō	ILE		29		30.951	-4.502	16.068		36.51			0
	MOTA	487	Ŋ	LEU		30		32.084	-2.715	15.617		44.61			N
35	ATOM	489	CA	LEU		30		31.023	-2.165	14.783		41.39			C
33	ATOM	491	СВ	LEU	A	30		31.284	-0.684	14.562		36.72			C C
	ATOM	494	CG	LEU	A	30		30.022	0.080	14.326		38.55			
	ATOM	496	CD1	LEU	A	30		29.865	1.229	15.255		44.29			C C
	ATOM	500	CD2	LEU	JA	30		30.137	0.569	12.982		43.51			C
40	ATOM	504	С	LEU	A	30		30.885	-2.911	13.455		40.85			0
	ATOM	505	0	LEC	A	30		31.851	-3.397	12.897		45.44			N
	ATOM	506	N	VAI	A	31		29.662		12.953		43.56			C
•	ATOM	508	CA	VAI	A	31		. 29.362		11.762		42.56			c
•	ATOM	510	CB	IAV	. A	31		28.116				44.28			C
45	ATOM	512		L VAI		31		27.424				46.25 48.98			Ċ
	MOTA	516	CG	2 VA1	LΑ			. 28.472				0 42.04			Ċ
	· MOTA	520	C		LΑ			29.137				0 46.43			ō
	MOTA	521	0		ĻΑ			28.088					· · .		N
٠.	MOTA	. 522	Ŋ		PΑ			30.113				0 38.37			C
50	ATOM	524	CA		PΑ		· · · ·	30.170				0 36.43 0 41.59	•		c
	MOTA	526	CB		ΡĀ			31.409			•	0 41.39			ç
	MOTA	529			P A			31.371			*	0 58.39	•		0:
,	MOTA	530		1 AS				30.241			•	0 38.39 0 43.43			0
	ATOM	531		2 AS				32.299				0 43.43 0 36.03			č
55	ATOM	532		AS	P A	32		30.308				0 36.03 0 36.16			ŏ
	ATOM	533				. 32		31.379				0 36.16 0 35.12		٠	N
	MOTA	534				. 33		29.238				0 36.24			C
	ATOM	536			R A			29.341				0 40.04			c
	MOTA	538			R A			27.969				0 44.25			ŏ
60	MOTA	540		1 TH				26.982				0 40.43			C
	ATOM	542	CG	2 TH	RA	33		27.453	3 -4.347	, 5.57		- 10.43			_

5	ATOM	546	С	THR A	33		29.829	-1.581	4.301	1.00 33.30			С
5	ATOM	547	0	THR A			29.893	-1.701	3.085	1.00 35.29		•	0
	ATOM	548	N	GLY A			30.177	-0.493	4.946	1.00 31.75			N
	ATOM	550	CA	GLY A			30.601	0.715	4.245	1.00 36.33			С
	ATOM	553	C	GLY A			32.077	0.844	4.160	1.00 39.91			С
10	ATOM	554	ō	GLY A			32.531	1.605	3.314	1.00 50.07			0
10		555	N	SER A			32.814	0.107	5.004	1.00 37.10			N
	MOTA	557	CA	SER A			34.228	0.032	4.901	1.00 34.40			. C
	ATOM	559	CB	SER A			34.823	0.796	6.021	1.00 36.88			С
	ATOM		OG	SER A			34.960	-0.016	7.136	1.00 40.38			0
1.5	ATOM	. 562 564	C	SER A			34.785	-1.406	4.922	1.00 37.08			С
15	MOTA			SER A			34.045	-2.332	5.176	1.00 32.07			0
	ATOM	565	0	SER A			36.104	-1.546	4.668	1.00 37.61			N
	MOTA	566	N	SER A			36.836	-2.824	4.521	1.00 38.67			C
	ATOM	,568 570	CA	SER F			37.384	-2.903	3.110	1.00 39.52			C
00	MOTA	570	CB				36.354	-2.718	2.156	1.00 47.74			0
20	ATOM	573	OG	SER A			38.079	-3.054	5.406	1.00 41.95			С
	MOTA	575	С	SER A			38.978	-3.850	5.074	1.00 42.44			0
	MOTA	576	0	SER A			38.162	-2.374	6.526	1.00 35.87			N
	MOTA	577	N	ASN A				-2.563	7.336	1.00 30.94			C
	MOTA	579	CA	ASN I			39.299		7.505	1.00 36.25			C
25	MOTA	581	CB	ASN A			39.969	-1.216	6.507	1.00 35.00			Ċ
	MOTA	584	CG	ASN A			41.020	-0.997	5.452	1.00 41.51			ō
	ATOM	585		ASN A			40.726	-0.519	6.819	1.00 35.89			N
	MOTA	586		ASN A			42.275	-1.379		1.00 30.50			C.
	MOTA	589	С	ASN A			38.876	-3.085	8.679	1.00 34.21			o
30	MOTA	590	0	ASN I			37.991	-2.530	9.247	1.00 34.21			N
	MOTA	591	N	PHE A			39.478	-4.157	9.184	1.00 36.14			. C
	MOTA	593	CA	PHE 1			39.180	-4.625	10.545	1.00 38.42			Č
	ATOM	595	CB	PHE 2			39.256	-6.146					č
	MOTA	598	CG	PHE 2			38.886	-6.678	12.040	1.00 43.00			c
35.	ATOM	599		PHE 2			39.713	-7.566		1.00 42.48 1.00 47.58			C
•	MOTA	601		PHE .			39.386	-8.040	13.962				c
	MOTA	603	CZ	PHE			38.233	-7.661	14.586	1.00 42.81			Ċ
	MOTA	605		PHE .			37.394	-6.785	13.954	1.00 49.46			c
	ATOM	607	CD2	PHE .			37.717	-6.290	12.670	1.00 44.85			Č
40	MOTA	609	С	PHE .			40.227	-3.888	11.416	1.00 40.18			o
	ATOM	610	0	PHE .			41.406	-3.760	11.017	1.00 39.66			41
	MOTA	611	N	ALA			39.802	-3.389	12.576	1.00 40.32			C
	MOTA	613	CA	ALA			40.656		13.403	1.00 40.28			Ċ
	MOTA	615	CB	ALA			40.810	_	12.739	1.00 40.18			C
45	ATOM .	619	C.	ALA		9	40.020		14.757	1.00 37.73			Ö
•	ATOM	620	0	ALA	A 3	9	38.787	-2.412	14.885	1.00 40.37			
	ATOM	.621	N	VAL	A 4	0	40.839		15.764	1.00 38.68			N
	MOTA	623	CA	VAL	A 4	0	40.334	-2.088	17.117	1.00 39.39			
	ATOM	625	ÇВ	VAL	A 4	0	40.369		17.636				. C
50	ATOM	627	CG1	VAL	A 4	0	39.731					•	C
	ATOM	631	CG2	VAL	A 4	0	41.722		17.829				. C
	ATOM	635	,C	VAL	A 4	0	41.080		18.005				C
	ATOM	636	0	VAL	A 4	0	42.175	-0.583	17.642		•		0
	ATOM	637	. N	GLY		1	40.477	-0.729	19.152				N
55	ATOM	639	CA			1	41.073	0.262	20.014				· C
33	ATOM	642	С	GLY		1	42.290		20.595				C
	ATOM	643		GLY		1	42.140		21.332				0
	ATOM	644	N	ALA		2	43.500		20.274				N
	MOTA	_		ALA		2	44.724		20.914	1.00 42.69			С
60 ·		648		ALA		2	45.655		19.886				С
00.	ATOM	652				12	45.444		21.883				С
	WI OLA	0.52	_	1		_							

_			_			40	4.0	6.687	0.515	21.984	1 00	45.43			0
5	ATOM	653	0	ALA		42			1.246	22.636		50.46			N
	ATOM	654	N	ALA		43		1.677		23.548		52.82			C
	ATOM	656	CA	ALA		43		5.278	2.216	22.854		48.10			Ċ
	ATOM	658	CB	ALA		43		5.320	3.073			56.62			č
	ATOM .	662	С	ALA		43		1.196	3.101	24.052		57.66			ō
10	MOTA	663	0	ALA		43		3.186	3.315	23.380					N.
	ATOM	664	N	PRO	Α	44		1.446	3.628	25.238		62.73			C
	ATOM	665	CA	PRO	Α	44		3.510	4.492	25.962		59.53			C
	ATOM	667	CB	PRO	Α	44		1.390	5.093	27.053		62.72			
	MOTA	670	CG	PRO	Α	44		5.835	4.754	26.603		66.12			C
15	ATOM	673	CD	PRO	A	44	4 :	5.696	3.411	26.003		65.12			C
	MOTA	676	·C	PRO	Α	44		2.905	5.606	25.132		59.62			C
	ATOM	677	0	PRO	Α	44	4	3.553	6.133	24.218		55.79	•		0
	ATOM	678	N	HIS	Α	45	4	1.653	5.939	25.452		54.87			N
	ATOM	680	CA-	HIS		45	4	0.970	7.043	24.813		54.75			С
20	ATOM	682	CB	HIS	Α	45	4	0.782	6.831	23.332		50.69			С
. 20	ATOM	685	CG	HIS		45	3:	9.905	7.860	22.704		47.13			С
	ATOM	686		HIS		45	3	8.634	8.126	23.167		46.73			N
•	MOTA	688		HIS		45	3	8.094	9.082	22.429		49.26			С
	ATOM	690		HIS		45	3	8.965	9.443	21.501		40.27			N
25	ATOM	692		HIS		45	4	0.108	8.692	21.654		46.25			C
23	ATOM	694	С	HIS		45	3	9.645	7.185	25.525		61.01			С
	ATOM	695.	ō	HIS		45	3	8.869	6.236	25.629		68.54			0
	MOTA	696	N	PRO		46	3	9.368	8.398	25.976		66.55	•		N
	ATOM	697	CA	PRO		46		8.316	8.630	26.973		67.17		•	С
30	ATOM	699	CB	PRO		46		7.953	10.103	26.772		67.46			С
30	ATOM	702	CG	PRO		46	3	9.078	10.729	25.902	1.00	64.56			С
	ATOM	705	CD	PRO		46		9.993	9.648	25.496	1.00	65.48			С
	MOTA	708	C	PRO		46		7.104	7.770	26.736		65.38	•		С
	ATOM	709	ō	PRO		46		6.433	7.311	27.650		68.92			0
35	ATOM	710	N.	PHE		47	•	6.823	7.530	25.479	1.00	62.71			N .
33.	ATOM	712	CA	PHE		47		5.613	6.833	25.156	1.00	60.29			С
	ATOM	714	СВ	PHE		47		5.137	7.330	23.806	1.00	58.61			С
	ATOM	717	CG	PHE		47		4.910	8.805	23.780	1.00	57.85			C
	ATOM	. 718		PHE		47		4.809	9.490	22.583	1.00	54.09			С
40	ATOM	720		PHE		47		4.602	10.831	22.559	1.00	50.97			С
40	ATOM	722	CZ	PHE		47		4.486	11.529	23.739	1.00	57.26			С
		724		PHE		47		34.583	10.865	24.944	1.00	60.84			C
	ATOM	726		PHE		47		34.792	9.507	24.965	1.00	59.30			С
	MOTA	728	C	PHE		47		35.728	5.340	25.155	1.00	58.83			С
45	MOTA	729	o	PHE		47		34.806	4.684	24.721	1.00	61.67			0
43	ATOM	730	N	LEC		48		36.829	4.774	•	1.00	58.46			N
	ATOM	732	CA	LEU		48		36.896	3.322		1.0	61.24			С
	MOTA	734	CB	LEU		48		38.084	2.812			59.23			C.
•	ATOM			LEU		48		38.037	3.121			60.91		-	C
50	ATOM	737	CG	l LEC		48		39.439	3.297		1.0	56.82			С
50	ATOM	739		2 LEC		48		37.235	2.074		1.0	61.09			С
	MOTA	743						36.928	2.709			0 62.47			С
	ATOM	747		LEU								0 61.13			0
	MOTA	748	0	LEU				37.767				0 65.56		. •	N
	MOTA	749		HIS				35.984				0 66.38		•	. с
55	ATOM	751	CA	HIS				36.036				0 73.64			c
•	ATOM	753			5 A			34.791				0 78.39			Ċ
	MOTA	756			5 A			33.560				0 87.79			N
	MOTA .	757		1 HIS				33.631				0 87.79			c
	MOTA	759		1 HIS				32.415							N
60	ATOM	761		2 HI	s A	. 49		31.550				0 84.81			C
	MOTA	763	CD	2 HI	s A	49		32.241	0.494	28.908	1.0	0 79.17			J

5	MOTA	765	С	HIS A	49		37.173	-0.070	28.366	1.00 60.95			C.
•	ATOM	766	Ö	HIS A	49		37.563	-0.684	29.362	1.00 60.23			0
	ATOM	767	N	ARG A	50		37.669	-0.304	27.149	1.00 58.11			N
	ATOM	769	CA	ARG A	50		38.768	-1.253	26.923	1.00 55.40			C
	ATOM	771	СВ	ARG A	50		38.247	-2.671	26.985	1.00 55.21			С
10			CG	ARG A	50	•	36.757	-2.807	26.821	1.00 54.36			С
10	MOTA	774	CD	ARG A	50		36.239	-4.211	27.167	1.00 48.77	•		С
	ATOM	777	7		50	٠	35.083	-4.540	26.350	1.00 52.02			N
	MOTA	780	NE	ARG A				-5.760	26.210	1.00 49.86			C
	MOTA	782	CZ	ARG A	50		34.594	-6.765	26.847	1.00 49.97			N
	ATOM	783		ARG A	50		35.170		25.440	1.00 44.75			N
15	MOTA	786		ARG A	50.	•	33.529	-5.971	25.631	1.00 56.08		•	c
	ATOM	789	С	ARG A	50		39.577	-1.078		1.00 55.23			ŏ
	ATOM	790	0	ARG A	50		39.388	-0.103		1.00 56.91			N
	MOTA	791	N	TYR A	51		40.506	-2.013	25.413	1.00 57.53			C
	MOTA	793	CA	TYR A	51		41.319	-2.010	24.195				c
20	ATOM	795	CB	TYR A	51		42.153	-0.735	24.085	1.00 58.76			c
	MOTA	798	CG	TYR A	51		43.220	-0.483	25.148	1.00 65.10			C
	MOTA	799·		TYR A	51		44.487	-1.041	25.057	1.00 70.53			
	ATOM	801	CE1	TYR A	51		45.460	-0.792	26.036	1:00 68.47			C
•	ATOM	803	CZ	TYR A	51		45.171	0.023	27.101	1.00 64.05			C
25	MOTA	804	OH .	TYR A	51		46.091	0.286	28.077	1.00 56.09			0
	MOTA	806	CE2	TYR A	51		43.947	0.573	27.198	1.00 65.65			C
	ATOM	808	CD2	TYR A	51		42.971	0.328	26.222	1.00 64.80			C
	ATOM .	810	C	TYR A	51		42.211	-3.222	24.026	1.00 56.08		٠.	C
•	MOTA	811	0	TYR A	51		42.650	-3.810	24.983	1.00 63.38			0
30	ATOM	812	N	TYR A	52		42.456	-3.600	22.783	1.00 56.18			N
•	MOTA	814	CA	TYR A	52		43.369	-4.698	22.440	1.00 54.65			Ċ
	MOTA	816	CB	TYR A	52		43.609	-4.634	20.954	1.00 52.23		-	C
	ATOM	819	CG	TYR A	52		44.309	-5.802		1.00 49.44			C
	MOTA	820		TYR A	52			-7.038	20.958	1.00 49.18	•		Ċ
35	ATOM	822		TYR A	52		45.014	-8.084	20.352	1.00 44.95			C
	MOTA	824	CZ	TYR A	52		45.598	-7.880	19.123	1.00 40.40			. C
•	ATOM	825		TYR A	52	•	46.257	-8.880	18.453	1.00 43.51			0
	ATOM	827		TYR A	52		45.543	-6.683	18.523	1.00 36.90			C
	MOTA	829		TYR A	52		44.906	-5.663	19.117	1.00 44.53			C
40	MOTA	831	С	TYR A	52		44.716	-4.512	23.090	1.00 56.76			C
	MOTA	832	0	TYR A	52		45.267	-3.421	23.042			,	0
	MOTA	833	N	GLN A	53		45.269	-5.562	23.694	1.00 58.49			N
•	ATOM	835	CA	GLN A	53		46.570	-5.444	24.371	1.00 50.39			C
	ATOM	837	CB	GLN A	53		46.443	-5.654		1.00 52.39			С
45	MOTA	840	CG	GLN A			45.728	-4.466	26.574	1.00 57.22			C
	ATOM	843	CD	GLN A	53		45.807	-4.475	28.089	1.00 59.21			C
	ATOM	844	OE1	GLN A	53		44.778	-4.523		1.00 68.21	•		0
	ATOM-	845	NE2	GLN A			47.019	-4.413	28.627	1.00 60.90			И
•	MOTA	848	С	GLN A	53		47.498	-6.427	23.723	1.00 48.79			C
50	MOTA	849	0	GLN A	53		47.660	- 7.571	24.144	1.00 48.67		-	0
	MOTA	850	N	ARG A	54		48.115		22.659	1.00 44.44			N
•	ATOM	852	CA	ARG A			48.994	-6.809	21.908	1.00 42.47			Ċ
	ATOM	854	CB	- ARG A			49.669	-5.949	20.864	1.00 42.10			C
	ATOM .	857	CG	ARG A	54		48.733	-5.430	19.740	1.00 35.73			С
55	ATOM	860	CD	ARG A			49.465	-4.449	18.787	1.00 38.01			С
	MOTA	863	NE	ARG A	•		49.506	-3.127		1.00 46.13			N
	ATOM	865	CZ	ARG A	54		50.064		18.861	1.00 54.49			. С
	ATOM	866		ARG A	54		50.646	-2.176	17.682	1.00 63.14			N
	ATOM	869		ARG A			50.052	-0.903		1.00 58.58			N
60	ATOM	872	С	ARG A			50.023	-7.562	22.802	1.00 46.11			С
-	ATOM	873	0	ARG A			50.297	-8.750	22.623	1.00 50.14			0

-		074 1	NT (GLN A	. 5	5		50.583	-6.	887	23.777		49.49			N
5	MOTA	-		GLN A		5		51.570	-7.	530	24.638	1.00	54.83			С
	MOTA			GLN A		5		52.120	-6.		25.638	1.00	56.89			С
	MOTA					55 .		51.331	-5.		25.639		63.64			C.
	ATOM			GLN A				50.389	-4.		26.815		69.23			С
	MOTA			GLN A		55		49.575	-4.		26.852		65.62			0
10	ATOM		OE1	GLN A		5					27.790	1.00	75.17			N
	MOTA			GLN F		5		50.502			25.379		56.17			С
	MOTA	889		GLN F		55		51.054			25.952		55.62			0
	MOTA	890		GLN A		55		51.849		509	25.388		55.53			N
	MOTA	891		LEU. A		66		49.750		047	26.133	1 00	56.08			С
15	ATOM	893	CA	LEU A		6		49.250					57.00		-	Ċ,
	MOTA	895	CB	LEU A		56		48.009		835	26.904	1.00	61.56			Ċ
	MOTA		CG	LEU A	-	56 _		48.155		608 .	27.785		62.62			Č
	MOTA	900	CD1	LEU A	A :	56		46.968		502	28.711					č
	ATOM	904	CD2	LEU A	A !	56		49.453		699	28.580		63.10			c
20	ATOM		С	LEU A		56		48.874	-11.	462	25.352		56.64			Ö
	MOTA		0	LEU Z	Α :	56		48.488	-12.	472	25.953		56.22			
•	ATOM		N	SER I		57	•	48.965	-11.	396	24.029		55.33			N
	ATOM	912	CA	SER		57		48.533	-12.	. 496	23.198		51.40			C
		914	СВ	SER		57		47.674	-12	.011	22 [.] .060		50.76			С
25	MOTA	917	OG	SER .		57		47.423			21.154		51.82			0.
23	ATOM	919	C	SER		57		49.768			22.633		54.74			С
	ATOM		0	SER		57		50.673			22.229	1.00	64.50			0
	ATOM	920	N	SER		58		49.827			22.582		51.36			N
	MOTA	921		SER		58		51.036	-14	. 980	22.152	1.00	52.68			С
	ATOM	923	CA	SER		58		51.243	-16	234	22:948	1.00	55.44			C.
30	ATOM	925	CB			58		50.240	-17	.142	22.588		51.95			. 0
	MOTA	928	OG	SER				50.913	-15	342	20.717		51.45			C,
	MOTA	930	С	SER		58		51.810	-15	932	20.154		58.22			0
	MOTA	931	0	SER		58		49.790			20.122		49.52			N .
	MOTA	932	N	THR		59		49.790			18.719		45.44			С
35	MOTA	934	CA	THR		59		48.187	-15	086	18.586		43.26	-		С
	MOTA	936	СВ	THR		59		47.220	-15	363	19.446		40.46	•		0
	MOTA	938		THR		59		47.220	17	366	19.192		43.84		•	С
	MOTA	940		THR		59		48.237	-17	. 000	17.894		48.17			С
	MOTA	944	С	THR		59		49.674	-13	001	16.676		49.26	•		0
40	. ATOM	945	0	THR		59 .		49.471	-13	. 901			3 44.42			N
	MOTA	946	N	TYR		60		50.023			18.556		0 45.38			C
	MOTA	948	CA	TYR		60		50.180			17.852		0 46.42			C
	MOTA	950	CB	TYR	Α	60		50.484			18.843		0 46.42			Ĉ.
	MOTA	953	CG	TYR	Α	60		50.852		182	18.198					
45	ATOM	954	· CD1	LTYR	Α	60		49.94		3.500	17.379		0 47.22		•	C C
	ATOM	956	· CE	L TYR	A	60		50.29		7.282	16.787	_	0 47.17			Ċ
	MOTA	958	CZ.	TYR	Α	60		51.54	-	5.741	17.003		0 44.65			. 0
	MOTA	959	OH	TYR	. A	60		51.89	4 -	5.538	16.408		0 49.47			
•	ATOM	961		2 TYR		60		52.44	8 - 3	7.393	17.813		0 41.96			C
50	ATOM	963		2 TYR		60		52.10	1 -1	3.604	18.408		0 45.55			C.
50	ATOM	.965	С	TYR				51.32	5 -1 ,	1.709	16.878		0 47.40			C
		966	Ö	TYR		60		52.26	2 -1	2.460	17.080		0 51.21			0
	ATOM	967	N.	ARG		61.		51.24	9 -1	0.942	15.804		0 48.35			N.
	ATOM					61		52.38	8 -1	0.781	14.920	1.0	0 41.23			C
	ATOM					61		52.39	2 -1	1.782	13.795	1.0	0 44.25			C
55	ATOM	971				61		52.53	8 -1	3.205			0 45.20			С
	ATOM	974						52.33	51	4.118			0 46.69			С
	MOTA	977				61		52 21	3 -1	5.391			0 51.89			N
	ATOM	980				61		50 00	2 _1	6.545	13.066		0 51.83			С
	MOTA	982				61		52.03 £1 07	10 -1	6.575	12.248		0 59.34			N
60	MOTA	983		1 ARG		61	•	DI.0/	0 _1	7.668			0 50.67			. N
	ATOM	986	NH	2 ARG	Αċ	61		55.44	0 -1	7.000	10.40.					

5	MOTA	989	С	ARG	Α	61		52.287	-9.433	14.302	1.00 4					С
	MOTA	990	0 .	ARG	A	61		51.278	-9.127	13.687	1.00					0
	MOTA	991	N	ASP	Α	62		53.374	-8.681	14.477	1.00					N
	ATOM	993	CA	ASP	Α	62		53.654	-7.322	13.990	1.00					C
	ATOM	995	CB	ASP	Α	62		54.947	-6.899	14.658	1.00					С
10	ATOM	998	CG	ASP	Α	62		55.158	-5.405	14.673	1.00 5					С
	ATOM	999	OD1	ASP	Α	62		54.562	-4.701	13.833	1.00	47.18				0
	ATOM	1000	OD2	ASP	A	62		55.940	-4.872	15.520	1.00	56.56				0
	ATOM	1001	С	ASP		62		53.950	-7.230	12.530	1.00	38.57				С
	ATOM	1002	0	ASP		62		54.868	-7.840	12.078	1.00					0
15	ATOM	1003	N	LEU		63		53.204	-6.429	11.784	1.00	42.04				N
	ATOM	1005	CA	LEU		63		53.464	-6.332	10.355	1.00	41.63			,	C
	ATOM	1007	СВ	LEU		63		52.131	-6.216	9.586	1.00	39.89				С
	ATOM	1010	CG	LEU		63		51.262	-7.490	9.430	1.00	39.13				С
	ATOM	1012		LEU		63		49.768	-7.233	9.242	1.00	38.98				С
20	ATOM	1016		LEU				51.755	-8.283	8.272	1.00	35.93				C .
20	ATOM	1020	C	LEU		63		54.414	-5.180	10.024	1.00	45.54				С
	ATOM	1021	ō	LEU		63		54.659	-4.921	8.853	1.00	45.94				0
	ATOM	1022	N	ARG		64		54.933	-4.467	11.034	1.00	47.05				N
	ATOM	1024	CA	ARG		64		55.873	-3.385	10.779	1.00					С
25	ATOM	1026	CB	ARG		64		57.261	-3.976	10.447	1.00					С
	ATOM	1029	CG	ARG		64		57.974	-4.717	11.615	1.00	48.68				С
	ATOM .	1032	CD	ARG		64		58.685	-6.010	11.233	1.00	49.84				С
	ATOM	1035	NE	ARG		64		59.846	-5.810	10.371	1.00	52.18				N
	MOTA	1037	·CZ	ARG		64		60.138	-6.547	9.301	1.00					С
30	ATOM	1038		ARG		64		59.360	-7.557		1.00					N
50	ATOM	1041		ARG		64		61.220	-6.268	8.594	1.00	59.82				N
	ATOM	1044	С	ARG		64		55.451	-2.492	9.608	1.00					С
	MOTA	1045	ō	ARG		64		56.259	-2.219	8.721	1.00	53.48				0
,	ATOM .	1046	N	LYS		65		54.198	-2.035	9.584	1.00			٠		N
35	ATOM	1048	CA	LYS		65		53.686	-1.175	8.489		51.33				С
<i>33</i> .	ATOM	1050	СВ	LYS		65		53.329	-2.050	7.229	1.00	•	• •			Ċ
•	ATOM	1053	CG	LYS		65		52.131	-1.667	6.219	1.00	48.91	•			С
	ATOM	1056	CD	LYS		65		51.911	-2.702	4.881	1.00	50.16				С
	ATOM	1059	CE	LYS		65		50.792	-4.019	4.900	1.00	44.00			•	С
40	ATOM	1062	NZ	LYS		65		51.193	-5.488	4.701	1.00	11.49				N
	ATOM	1066	C	LYS		65		52.519	-0.436	9.136	1.00	50.12				С
	ATOM	1067	0	LYS		65		51.705	-1.075	9.781	1.00	56.99				0
	MOTA	1068	N	GLY		66		52.450	0.890	9.005	1.00	47.93				N
	ATOM	1070	CA	GLY		66		51.359	1.678	9.588	1.00	45.56				С
45	ATOM	1073	С	GLY		66		50.196	1.971	8.628	1.00	42.47				С
:-	ATOM	1074	0	GLY		66		50.277	1.787	7.418	1.00	40.89				0
	ATOM	1075	N	VAL		67		49.095	2.470	9.152	i.00	39.98			•	N
•	ATOM	1077	- CA	VAL		67		48.000	2.820	8.264		35.53				С
	ATOM	1079	СВ	VAL		67		47.307	1.531	7.793		35.43	•			С
50	MOTA	1081		VAL		67		46.878	0.663	8.984		36.95				С
30	ATOM	1085		VAL		67		46.129	1.806	6.999		33.52				С
	MOTA	1089	C			67		47.021		8.882		40.42				С
	MOTA	1090		VAL		67		46.885	3.969			40.64				0
. ,	ATOM	1091	N.			68		46.352		7.971		45.72		:		N.
55	MOTA	, 1093	CA	TYR		68		45.436				46.34		٠.		C.
55	ATOM	1095		TYR		68		46.052	6.874	7.536		51.19	•	•		, C
•		1098	CG			68		45.306		7.533		61.31				C
	MOTA	1098		TYP		68		44.911	8.826	8.726		62.21			•	C
	ATOM ATOM	1101		TYF		68		44.266	10.043	8.702		61.39				Ċ
60			CZ	TYF		68		44.200	10.665	7.491		63.25				c
50	MOTA	1103				68		43.361	11.886	7.472		66.32				ō
	MOTA	1104	OH	TYF	, n	00	2	42.20I	11.000	1,716	1.00	00.52				-

5	MOTA	1106	CE2	TYR A	. 68		44.390	10.080	6.298	1.00 58.19			С
-	ATOM	1108	CD2	TYR A	68		45.039	8.864	6.321	1.00 61.27	• •		С
	ATOM	1110	С	TYR A	68		44.152	5.440	7.505	1.00 41.55		•	C
		1111	0	TYR A			44.130	5.185	6.335	1.00 42.23			0
	ATOM		N	VAL A			43.045	5.557	8.195	1.00 45.73			N
10.	· ATOM	1112					41.791	5.348	7.519	1.00 43.18	•		С
10	MOTA	1114	CA	VAL A					7.920	1.00 46.99			Ċ
	MOTA	1116	CB	VAL A			41.256	3.958	•	1.00 46.87			Ċ.
	MOTA	1118		VAL A			39.856	3.712	7.399				č
	ATOM	1122		VAL A			42.216	2.897	7.399	1.00 39.84			c
	MOTA	1126	С	VAL A	69		40.831	6.478	7.832	1.00 37.88			
15	MOTA	1127	0	VAL A	69		40.436	6.622	8.962	1.00 45.27			0
	ATOM	1128	N	PRO A	70		40.497	7.286	6.823	1.00 34.02			N
	ATOM	1129	CA	PRO A	70		39.507	8.345	6.917	1.00 29.99			С
	ATOM	1131	CB ·	PRO A	70	•	40.071	9.345	5.934	1.00 26.73			С
•	ATOM	1134	CG	PRO A			40.414	8.518	4.800	1.00 25.36			C
20	ATOM	1137	CD	PRO A			41.047	7.267	5.456	1.00 34.53			С
20		1140	C	PRO A			38.118	7.941	6.383	1.00 35.42			С
	ATOM			PRO A			37.992	7.309	5.318	1.00 35.66			0
•	MOTA	1141	0				37.067	8.315	7.102	1.00 43.55			N
	MOTA	1142	N	TYR A						1.00 47.40	•		C
~~	ATOM	1144	CA	TYR A			35.699	8.076 7.305	7.684	1.00 48.07			č
25	MOTA	1146	CB	TYR A			34.943			1.00 49.56			Č
	MOTA	1149	CG	TYR A			35.651	6.025	8.159				c
	ATOM	1150	CD1	TYR A			35.181	4.750	7.818	1.00 49.21			
	MOTA	1152	CE1	TYR A			35.822	3.609	8.258	1.00 46.98			C
	MOTA	1154	CZ	TYR A			36.924	3.741	9.045	1.00 44.80		•	С
30	MOTA	1155	OH	TYR A	71		37.601	2.666	9.526	1.00 46.04			0
	MOTA	1157	CE2	TYR A	71		37.387	4.972	9.389	1.00 50.64			С
	MOTA	1159	CD2	TYR A	71		36.756	6.097	8.949	1.00 50.58			С
٠.	ATOM	1161	С	TYR A			34.974	9.409	6.253	1.00 51.01			С
	MOTA	1162	ō	TYR A			35.607	10.448	6.041	1.00 56.69			О
35	ATOM	1163	N	THR A			33.653	9.373	6.144	1.00 54.06			N
55	ATOM	1165	ĊA	THR A			32.842	10.586	5.982	1.00 48.48	•		С
		1167	СВ	THR A			31.462	10.140	5.541	1.00 42.95			С
•	ATOM	1169	OG1				31.614	9.334	4.387	1.00 44.35			O
	MOTA			THR A			30.620	11.232	4.935	1.00 46.38			Ċ
40	MOTA	1171					32.834	11.426	7.291	1.00 50.73			Č
.40	MOTA	1175	C	THR A			32.793	12.633	7.256	1.00 49.87			ō
	MOTA	1176	0	THR A				10.790	8.446	1.00 57.02			N
	MOTA	1177	N	GLN A			32.873				•		c
	ATOM	1179	CA	GLN A			33.020	11.507	9.717	1.00 61.36			C
	MOTA	1181	CB	GLN A			31.704	11.705	10.489	1.00 61.87			С
45	MOTA	1184	CG	GLN A			30.932	13.008	10.237	1.00 69.07			
	MOTA	1187	CD	GLN A			31.616	14.250	10.830	1.00 73.52			С
	ATOM	1188		GLŅ A			31.469	14.561	12.028	1.00 73.43			0
	ATOM	1189	NE2	GLN A			32.369	14.960	9.987	1.00 74.63			N
	MOTA	1192	С	GLN I	A 73		33.930	10.654	10.576	1.00 61.53			С
50	MOTA	1193	0	GLN A	A 73		33.592	9.520	10.910	1.00 63.25			- 0
	ATOM	1194	N	GLY A			35.079	11.208	10.935	1.00 62.04			N
	ATOM	1196	CA	GLY A			36.019	10.538	11.816	1.00 60.66	•.		Ċ
	ATOM	1199	C	GLY I		:	37.207	9.927	11.093	1.00 54.01		٠.	Ċ
:		1200	ó	GLY A		• •	37:126	9.641	9.901	1.00 47.51			.0
55	MOTA						38.310		11.822	1.00 51.55	. :		N
55	MOTA	1201	N	LYS A		•			11.330	1.00 48.56			C
	MOTA	1203		LYS A			39.445						c
•	MOTA	1205	СВ	LYS A		-	40.395		10.472	1.00 49.33			C
	MOTA	1208	CG	LYS A			40.953		11.076	1.00 50.33			
	MOTA	1211	CD	LYS A			41.467		9.917	1.00 49.25			C
60	MOTA	1214	CE	LYS A		•	41.609		10.286	1.00 50.50			C
	MOTA	1217	NZ	LYS A	A 75		43.031	13.815	10.654	1.00 42.60			N
		•											

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5	ATOM	1221	С	LYS	Α	75		40.203	8.425	12.455	1.00 45.8			C	
•	ATOM	1222	0	LYS	Α	75		39.958	8.795	13.599	1.00 46.4			0	
	ATOM	1223	N	TRP	A	76		41.105	7.501	12.110	1.00 46.3			N	
	ATOM	1225		TRP		76		42.052	6.881	13.058	1.00 47.2			C	
	MOTA	1227	CB	TRP	A	76		41.502	5.620	13.777	1.00 41.9			C	
10	ATOM	1230		TRP		76		40.864	4.653	12.875	1.00 40.5			C	
	MOTA	1231	CD1	TRP	Α	76		39.552	4.578	12.592	1.00 42.4				
	ATOM	1233		TRP		76		39.304	3.557	11.706	1.00 44.2			N	
·	MOTA	1235	CE2	TRP	Α	76		40.488	2.949	11.407	1.00 40.3			C	
	ATOM	1236	CD2	TRP	A	76		41.494	3.615	12.132	1.00 39.7			C	
15	ATOM	1237	CE3	TRP	Α	76		42.814	3.176	11.996	1.00 43.2		•	C	
••	ATOM	1239	CZ3	TRP	Α	76		43.082	2.116	11.157	1.00 34.0			C	
	ATOM	1241	CH2	TRP	A	76		42.047	1.481	10.452	1.00 40.8			C	
	ATOM	1243		TRP		76		40.749	1.887	10.567	1.00 37.4			C	
•	MOTA	1245	C.	TRP	A	76		43.352		12.283	1.00 46.6			. С	
20	ATOM	1246	0	TRP	A	76		43.376	6.593	11.058	1.00 44.5			0	
	ATOM	1247	N	GLU-		77		44.417	6.302	13.025	1.00 44.4			N	
	ATOM	1249	CA	GLU	A	.77		45.726	6.056	12.465	1.00 49.			C	
	MOTA	1251	CB	GLU		77		46.637	7.292	12.696	1.00 54.			C	
	ATOM	1254	CG	GLU		77		45.798	8.559	12.966	1.00 63.			C	
25	MOTA	1257	CD	GLU		77		46.260	9.861	12.296	1.00 65.		•	C	
	ATOM	1258	OE1	GLU	Α	77		47.499	10.099	12.217	1.00 62.			0	
	ATOM	1259		GLU		77		45.341	10.642	11.855	1.00 57.			0	
	ATOM	1260	C	GLU		77		46.145	4.851	13.268	1.00 48.		•	C	
	ATOM	1261	0	GLU		77		45.835	4.787	14.477	1.00 46.			0	
30	ATOM	1262	N	GLY		78		46.814	3.881	12.643	1.00 44.			N	
50	ATOM	1264	CA	GLY	Α	78		47.148	2.670	13.387	1.00 43.			C	
	ATOM	1267	С	GLY		78		48.378	1.905	12.935	1.00 45.			C	
	ATOM	1268	.0	GLY	Α	78		49.054	2.322	11.945	1.00 46.			C	
•	ATOM	1269	N	GLU		79		48.635	0.805		1.00 40.			N	
35	ATOM	1271	CA	GLU	Α	79		49.702	-0.144	13.391	1.00 45.			C	
	ATOM	1273	CB	GLU	Α	79		50.631	-0.248	14.675	1.00 51.			C	
	ATOM	1276	CG	GLU	Α	79		51.478	1.000	15.101	1.00 55.				
	ATOM	1279	CD	GLU	Α	79		52.047	0.912	16.565	1.00 65.				
	ATOM	1280	OE1	GLU	Α	79		52.921	1.815	17.021	1.00 64.			C	
40	MOTA	1281	OE2	GLU	A	79		51.612	-0.082	17.271	1.00 54.			C	
	MOTA	1282	С	GLU	Α	79		49.162	-1.565	12.952	1.00 44.				2
	ATOM	1283	0	GLU	Α	79		48.318	-2.183	13.626	1.00 39.				C
	MOTA	1284	N	LEU	Α	80		49.666	-2.080	11.829	1.00 45.				N
	MOTA	1286	CA	LEU	ΙΑ	80		49.240	-3,386	11.250	1.00 42.				C
45	MOTA	1288	CB	LEU	A	80		49.454	-3.355	9.743	1.00 39.				С
	MOTA	1291	CG	LEU	J A	80		48.461	-2.502	9.024	1.00 38.				C
	ATOM	1293	· CD1	LEU	JA	80		48.671		7.556	1.00 41.		•		C
	ATOM	1297	CD2	LEU	JA	80		47.097	-2.967	9.427	1.00 43.		•		C
	ATOM	1301	ĊĹ	LEU				49.908	-4.689		1.00 42				C
50	ATOM	1302	.0.	LEC	JA	80		51.133	-4.789		1.00 39				0
	ATOM	1303	N	GL	ζA	81		49.084	~5.715		1.00 38				N
	ATOM	1305	CA	GL	ζĄ	81		49.519	-6.972						С
	ATOM	1308	С	GLY	ζA	81	•	48.517	-8.073						C
	MOTA	1309		GL				47.680	-7.948		1.00 40				0
55	ATOM	1310		THE				48.631	-9.167						N
	ATOM	1312						47.663	-10.265	12.824					C
	ATOM	1314		TH				48.071	-11.342	11.837					C
	ATOM	1316		1 TH				49.268	-12.009	12.302					0
	ATOM	1318		2 TH				48.423	-10.774	10.506					C
60	ATOM	1322			R A			47.570	-10.947	14.176					C
55	ATOM	1323				82		48.416	-10.779	15.077	1.00 41	.59			0
			_						•						

5	ATOM	1324	N	ASP	A	83		46.532	-11.736	14.315	1.00	39.43			N
	MOTA	1326	CA	ASP		83			-12.449	15.538		41.41			С
	MOTA	1328	CB	ASP		83			-11.482	16.675	1.00	40.00			С
	MOTA	1331	CG	ASP		83			-12.135	18.011		44.18			С
	MOTA	1332		ASP		83		46.475	-13.344	18.014	1.00	45.61			0
10	AT:OM	1333	OD2	ASP	Α	. 83		46.225	-11.551	19.111	1.00	52.07			0
	MOTA	1334	С	ASP	Α	83		45.163	-13.314	15.246	1.00	44.90			С
	ATOM	1335	0	ASP	Α	83		44.544	-13.136	14.216	1.00	51.63			Ó
	MOTA	1336	N	LEU	A	84		44.847	-14.260	16.110	1.00	45.58			'N
	ATOM	1338 0	···· CA	LEU	A	84		43.699	-15.139	15.877	1.00	44.62			С
15	ATOM	1340	CB	LEU	A	84.		43.951	-16.446	16.629	1.00	41.76		. *	С
	MOTA	1343	CG	LEU	Α	84		45.078	-17.361	16.133	1.00	41.81			C
	ATOM	1345	CD1	LEU	A	84		45.177	-18.491	17.103	1.00	46.46			С
	ATOM	1349	CD2	LEU		84		44.847	-17.978	14.767	1.00	42.92			. C
•	MOTA	1353	С	LEU	Α	84		42.374	-14.468	16.315	1.00	41,20			С
20	ATOM	1354	0	LEU	Α	84		42.388	-13.643	17.191	1.00	52.36			0
	MOTA	1355	N	VAĹ	Α	85		41.234	-14.803	15.719	1.00	41.48			N
	ATOM	1357	CA	VAL	A	85		39.973	-14.143	16.080	1.00	37.87			С
	ATOM	1359	CB	VAL	Α	85		39.743	-12.994	15.120	1.00	41.53			С
	MOTA	1361	CG1	VAL	A	85		38.437	-12.345	15.380	1.00	47.66			С
25	ATOM	1365	CG2	VAL	Α	85		40.822	-11.985	15.229	1.00	41.79			C
	MOTA	1369	C	VAL	A	85		38.680	-14.998	16.052	1.00	39.48		•	С
	MOTA	1370	.О	VAL	A	85		38.448	-15.737	15.125	1.00	44.43			Ó
	MOTA	1371	N·	SER	A	86		37.833	-14.882	17.068	1.00	40.31			N
	MOTA	1373	CA	SER	Α	86		36.564	-15.608	17.085		44.63		_	C
30	MOTA	1375	CB	SER	Α	86		36.474	-16.510	18.316		41.82		٠.	C
	ATOM	1378	OG	SER	Α	86			-17.097	18.545		55.30	•		0
	ATOM	1380	. C -	SER	Α	86		35.365	-14.678	17.157	1.00	45.48			С
	ATOM .	1381	Ο.	SER	A	86		35.525	-13.486	17.463		41.16			0.
	MOTA	1382	N	ILE	Α	87			-15.266	16.888		43.04			N
35	ATOM	1384	CA	ILE	Α	87			-14.643	17.083		41.10			С
	MOTA	1386	CB	ILE	A	87 .	***		-14.421	15.706		42.65			С
	MOTA	1388	CG1	ILE	Α	87			-13.839	14.754		43.78			C
	MOTA	1391	CD1	ILE	A٠	87		32.624	-13.331	13.496	1.00	47.44			С
	MOTA	1395	CG2	ILE	Α	87		31.050	-13.435	15.795	1.00	39.53			С
40	MOTA	1399	C	ILE	Α	87		32.022	-15.517	18.062	1.00	43.32			С
	MOTA	1400	0	ILE	Α	87		31.287	-16.462	17.663	1.00	44.61			0
	MOTA	1401	N	PRO	Α	88		32.120	-15.212	19.346		41.82			N
	MOTA	1402	CA	PRO	Α	88		31.440	-16.004	20.380	1.00	45.42			C
	MOTA	1404	CB	PRO	A	88		31.311	-15.040	21.563	1.00	46.34			C
45	MOTA	1407	CG	PRO	Α	88		-32.594	-14.147	21.446	1.00	46.41			С
	MOTA	1410	CD	PRO	A	88		32.902	-14.107	19.925		46.82		•	С
	MOTA	1413	.C	PRO		88		30.103	-16.508	19.949	i.00	44.85			С
	ATOM	1414	0	PRO	Α	88		29.867	-17.685	20.208	1.00	53.97			. 0
	MOTA	1415	N	HIS	Α	89		29.243	-15.692	19.354		46.76			N
50	MOTA	1417	CA	HIS	Ą	89		27.981	-16.214	18.801		50.05			С
	ATOM	1419	CB	HIS	A	89		26.757	-15.526	19.316		48.45			С
	MOTA	1422	CG _.	HIS	Α	89			-15.317	20.780		55.56			С
	ATOM	1423	ND1	HIS	Α	89	•		-16.302			60.41			N
	MOTA	1425	CE1	HIS	A ·	89			-15.830	22.899		64.25			·C
55	MOTA	1427		HIS		89			-14.576	22.842		59.22			N
	ATOM	1429		HIS		89			-14.229	21.524		56.69			C
	ATOM	1431	С	HIS		89	•		-15.966	17.339		54.03		٠.	c
	ATOM	1432	0	HIS		89			-15.179	16.853		55.54			ō
	ATOM'	1433		GLY		90			-16.606	16.653		55.69			N
60	ATOM	1435	CA	GLY		90	•		-16.585	15.201		55.66			C .
	ATOM	1438	C	GLY		90			-18.001	14.865		52.28			C
			-					22.40!	10.001	19.000	~.00	JZ.Z0			C

_			_	CT V A	90	29.482 -18.847 15.746 1.00 62.08	0
5	ATOM	1439	1	GLY A	91	29.704 -18.297 13.628 1.00 47.23	N
	ATOM	1440		PRO A		30.069 -19.664 13.308 1.00 47.93	С
	ATOM	1441	CA	PRO A	91	30.399 -19.586 11.830 1.00 49.04	С
	MOTA	1443	CB	PRO A	91 91	30.611 -18.114 11.561 1.00 45.67	С
	ATOM	1446	CG	PRO A	91	29.727 -17.419 12.456 1.00 48.30	С
10	MOTA	1449	CD	PRO A	91	31.248 -19.980 14.206 1.00 54.34	С
	MOTA	1452	C	PRO A		32.052 -19.090 14.448 1.00 56.82	0
	MOTA	1453	0	PRO A	91	31.343 -21.211 14.691 1.00 54.83	N
	MOTA	1454	N	GLN A	92	32.261 -21.569 15.765 1.00 55.86	С
	ATOM	1456	CA	GLN A	92	31.662 -22.754 16.503 1.00 60.18	С
15	MOTA	1458	CB	GLN A	92	30.322 -22.429 17.101 1.00 58.46	С
	ATOM	1461		GLN A	92	30.470 -21.890 18.493 1.00 64.81	С
	MOTA	1464	CD	GLN A	92	30.847 -22.631 19.418 1.00 63.91	0
	MOTA	1465		GLN A	92	30.178 -20.591 18.662 1.00 67.59	. N
	MOTA	1466		GLN A	92	33.635 -21.950 15.325 1.00 56.89	С
20	MOTA	1469	С	GLN A	92 03	34.036 -23.111 15.411 1.00 62.48	0
	ATOM	1470	0	GLN · A	92	34.387 -20.961 14.897 1.00 55.14	N
	MOTA	1471	N	VAL A	93	35.629 -21.223 14.237 1.00 50.07	. С
	MOTA	1473	CA	VAL A	93	35.426 -21.112 12.760 1.00 51.39	С
	ATOM	1475	CB.	VAL A	93	34.450 -22.169 12.285 1.00 53.66	,C
25	MOTA	1477		VAL A		34.902 -19.715 12.424 1.00 53.54	C
	MOTA	1481		VAL A	93	36.605 -20.174 14.620 1.00 54.79	C
	MOTA	1485		VAL A	93	36.303 -19.243 15.382 1.00 56.10	0
	MOTA	1486	.0	VAL A	93	37.805 -20.303 14.089 1.00 53.29	N
	MOTA	1487	N	THR A	94	38.802 -19.378 14.467 1.00 52.14	Ć
30	ATOM .	1489	CA	THR A	94	39.464 -19.960 15.690 1.00 53.16	С
	ATOM ,	1491	CB	THR A	94 94.	38.506 -19.888 16.761 1.00 53.79	О
	MOTA	1493		THR A		40.645 -19.093 16.197 1.00 56.24	С
	MOTA	1495		THR A	94 94	39.688 -19.131 13.285 1.00 52.21	С
0.5	MOTA	1499	C	THR A	94	40.148 -20.051 12.624 1.00 61.76	0
35	ATOM	1500		THR A	95	39.923 -17.867 12.993 1.00 51.10	N.
	ATOM	1501	N Cri	VAL A	95 95	40.645 -17.543 11.772 1.00 48.01	С
	ATOM	1503	CA	VAL A	95	39.722 -16.862 10.706 1.00 43.19	С
	MOTA	1505		VAL A		38.322 -17.270 10.858 1.00 37.56	С
á o	ATOM	1507		VAL A		39.760 -15.377 10.824 1.00 47.32	С
40	MOTA	1511	C	VAL A		41.736 -16.577 12.111 1.00 45.91	С
	MOTA	1515		VAL A		41.608 -15.811 13.065 1.00 50.89	0
	MOTA	1516	0	ARG A		42.814 -16.615 11.353 1.00 41.67	N
	ATOM	1517	N CA	ARG A		43.788 -15.565 11.502 1.00 43.07	С
AE	MOTA	1519	CB	ARG A		45.180 -16.043 11.235 1.00 41.47	С
45	ATOM	1521	CG	ARG A		46.175 -14.982 11.546 1.00 41.13	С
	ATOM	1524 1527	CD	ARG A		47.579 -15.400 11.409 1.00 43.93	C
	MOTA	1530				48.156 -15.492 12.744 1.00 52.62	. N
	MOTA			ARG A		48.450 -16.621 13.334 1.00 56.20	C
£0.	MOTA	1532		1. ARG A		48.233 -17.778 12.696 1.00 59.54	N
50	MOTA.			2 ARG A		48.965 -16.594 14.565 1.00 58.71	N
	ATOM	1536		ARG A	_	43.441 -14.460 10.512 1.00 40.12	С
	MOTA	1539				43.081 -14.756 9.368 1.00 46.93	. 0
	MOTA	1540		ARG A		43.539 -13.208 10.963 1.00 37.94	N
	ATOM	1541				43.294 -12.033 10.119 1.00 40.48	С
55	MOTA	1543				41.818 -11.575 10.255 1.00 40.89	С
	ATOM	1545		ALA A		44.193 -10.823 10.362 1.00 38.63	С
	MOTA	1549		ALA A		44.823 -10.673 11.393 1.00 40.23	0
	MOTA	1550				44.208 -9.957 9.358 1.00 41.67	N
	ATOM	1551		ASN A		44.823 -8.658 9.427 1.00 39.41	C
60	ATOM	1553				44.680 -7.992 8.094 1.00 42.95	. С
	MOTA	1555	5 CE	B ASN	א אַס	12.000	

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5 .	MOTA	1558		ASN A	98	45.476	-8.649	7.070		37.46 37.53			C 0
٠	MOTA	1559		asn a	98	46.593	-8.980	7.320		52:61			N
	ATOM	1560		asn a	98	44.915	-8.841	5.896		40.10			C
	ATOM	1563		ASN A	98	44.083	-7.799	10.369		41.02			Ö
	MOTA	1564		asn a		42.863	-7.864	10.434		44.12			N
10	MOTA	1565		ILE A		44.808	-6.962	11.089		44.12			C
	MOTA	1567		ILE A		44.198	-6.153	12.128		41.75			c
	MOTA	1569		ILE A		44.298	-6.840	13.502		43.97			Č
	ATOM	1571		ILE A		43.507	-8.127	13.511		48.22			c
	MOTA	1574		ILE A		43.588	-8.918	14.872		45.32			c
15	MOTA	1578		ILE A		43.722	-5.928	14.602		44.51			č
	ATOM	1582	-	ILE A		44.932	-4.844	12.154		47.40			Ö
	MOTA	1583		ILE A		46.082	-4.777	11.783 12.579		45.36			N
	ATOM	1584		ALA A		44.252	-3.795			41.65			C
•	ATOM	1586		ALA A		44.880	-2.510	11.762		41.33			Č
20	MOTA	1588	_	ALA A		44.230	-1.553	14.054					Ċ
	MOTA	1592	С	ALA A		44.732	-2.068	14.531	1 00	41.57			ō
	ATOM	1593	0	ALA A		43.612	-1.861	14.736		40.77			N
	ATOM	1594		ALA A		45.865	-1.951	16.066		37.99			C
	MOTA	1596	CA	ALA A		45.801	-1.461 -1.896	16.841		44.45			Ċ
25	MOTA	1598	CB	ALA A		46.907	0.007			41.73			C
	MOTA	1602	С	ALA A		45.819	0.611	15.432		40.15			Ō
. ,	ATOM	1603	0	ALA P		46.801	0.544	16.204		42.71			N
	ATOM	1604	N	ILE A		44,656 44.379	1.911	16.241		39.72			С
	MOTA	1606	CA	ILE A		43.010	2.009	16.549		44.46			С
30	ATOM	1608	CB	ILE F	102	42.182	1.767	15.321		43.48			С
	MOTA	1610		ILE A		40.768	1.961	15.644		40.40			С
	MOTA	1613 1617		ILE A		42.732	3.406	17.111	1.00	48.29			С
	ATOM ATOM	1621	.C		A 102	45.024	2.449	17.452		44.91		*	С.
35	ATOM	1622			A 102	44.777	1.856	18.522		42.30			0
JJ ,	MOTA	1623	N		A 103	45.795	3.544	17.257		45.74			N
	ATOM	1625	CA		A 103	46.583	4.269	18.265		48.02			С
	ATOM	1627	СВ	THR A	A 103	48.113	4.118	17.971		48.61			С
	ATOM	1629	OG1	THR I	A 103	48.365	4.329	16.578		53.38			0
40	ATOM	1631	CG2	THR A	A 103	48.601	2.733	18.209		42.44			С
• • •	ATOM	1635	C	THR 2	A 103	46.295	5.790	18.383		48.94			C O
	MOTA	1636	0		A 103	46.547	6.358	19.407		51.09			
	ATOM	1637	N	GLU .	A 104	45.804	6.456	17.343		54.39			N C
	MOTA	1639	CA	GLU .	A 104	45.357	7.855	17.474		56.21			C
45	ATOM	1641	CB	GLU .	A 104	46.402	8.823	16.940		61.91			c
	MOTA	1644	CG		A 104	47.736	8.206	16.593	• •	66.58			Č
	- ATOM	1647	CD		A 104	48.599	9.142	15.758		71.04 0 69.31			ŏ
	ATOM	1648			A 104	48.030							ŏ
	MOTA	1649	OE2		A 104	49.833	9.228	16.037		0 69.74			č
50	MOTA	1650	С		A 104	44.062				0 53.27			Ö
	ATOM	1651	0		A 104	43.890				0 44.69			N
	ATOM	1652	N		A 105	43.182		17.179	•	0 52.49	•		· C
	MOTA	1654			A 105	41.858				0 54.80			c
	MOTA	1656			A 105	40.954				0 53.62 0 51.12			ŏ
55	ATOM	1659			A 105	41.288				0 56.75			č
	ATOM	1661			A 105	41.136				0 55.75			0.
	ATOM	1662			A 105	41.285				0 57.71			N
	MOTA	1663			A 106	40.301				0 57.67			C
	MOTA	1665			A 106	39.596				0 60.33			č
60		1667			A 106	40.343 39.862				0 66.40			Ċ
	MOTA	1670	CG	· ASP	A 106	37.002	. 14.502	. 13.030		- 550			

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5	MOTA	1782 CA	SER A 113	29.408	4.080	21.174	1.00 60.39		С
		1784 CB	SER A 113	30.773	4.180	21.514	1.00 59.53		0
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	MOTA	1789 C	SER A 113	28.687	1.528	22.279	1.00 53.79		0
	MOTA	1790 0	SER A 113	27.891	1.879	23.613	1.00 48.58		N
10	ATOM	1791 N	ASN A 114	29.642	0.505	24.026	1.00 47.72		С
	MOTA	1793 CA	ASN A 114	29.882	-0.222	24.481	1.00 52.15		C
	MOTA	1795 CB	ASN A 114	28.660	-1.423	25.395	1.00 61.51		С
	ATOM ·	1798 CG	ASN A 114	29.015	-1.259	26.544	1.00 64.39		0
	ATOM		ASN A 114	29.436	-2.632	24.867	1.00 65.83		N
15	MOTA	1800 ND2	2 ASN A 114	28.867	-0.364	23.028	1.00 50.29		C
	ATOM	1803 C	ASN A 114	30.664	-1.544	23.314	1.00 51.67		0
	MOTA	1804 0	ASN A 114	30.981	0.204	21.871	1.00 48.89		N ·
•	MOTA	1805 N	TRP A 115	31.014	-0.536	20.929	1.00 46.17		С
	ATOM	1807 CA	TRP A 115	31.822	-0.530	19.518	1.00 42.77		C
20	ATOM	1809 CB	TRP A 115	31.244		18.828	1.00 39.20		Ċ
	MOTA	1812 CG	TRP A 115	30.907	0.748	18.787	1.00 35.62		С
	ATOM	1813 CD	1 TRP A 115	29.722	1.338	18.028	1.00 36.54		N
	MOTA	1815 NE	1 TRP A 115	29.782	2.481	17.575	1.00 33.32		С
	ATOM	1817 CE	2 TRP A 115	31.055			1.00 36.65		С
25	ATOM	1818 CD	2 TRP A 115	31.783	1.553	18.053 17.723	1.00 37.81		С
20	MOTA	1819 CE	3 TRP A 115	33.132	1.462		1.00 32.70		С
-	ATOM	1821 CZ	3 TRP A 115	33.681	2.419	16.946 16.485	1.00 43.43		С
	ATOM	. 1823 CH	2 TRP A 115	32.924	3.479	16.403		•	С
	ATOM	1825 CZ	2 TRP A 115	31.607	3.604				C
30	ATOM	1827 C	TRP A 115	33:277	-0.054				Ο.
50	ATOM	1828 O	TRP A 115	33.541	0.928				ที
	ATOM	1829 N	GLU A 116	34.204	-0.729				C
	MOTA	1831 CA		35.607	-0.389				c
•	ATOM	1833 CE	GLU A 116	36.192	-1.236				С
35	ATOM	1836 CG		35.916	-0.715				. C
-	MOTA	1839 CI		34.979	-1.591				0
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	MOTA	1841 OF	E2 GLU A 116	34.941	-2.830				С
	MOTA	1842 C	GLU A 116	36.444	-0.607				0
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•	MOTA	1844 N		35.754					С
	ATOM	1846 C		36.435					C
	ATOM	1849 C	GLY A 117	35.469					0
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45		1851 N		35.999					C
	MOTA	1853 C	A ILE A 118	35.113					С
	ATOM	1855 C		35.323	·				Ç
	ATOM	1857 C	G1 ILE A 118	34.441					C
	ATOM	1860 C	D1 ILE A 118	34.304					С
50		1864 C	G2 ILE A 118	36.669					С
-	MOTA	1868 · C		35.465					. 0
•	ATOM			36.608				•	N
	ATOM	1870 N	LEU A 119	34.445				•	C
	ATOM		CA LEU A 119	34.628					
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,,,	MOTA	1877	CG LEU A 119	33.96					C
	MOTA	- 1879	CD1 LEU A 119	35.43					Ċ
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60			O LEU A 119	32.96					N
J.C	ATOM	TIII 1	N GLY A 120	35.05	9 -3.7	94 9.0	J T.UU 40.20		
	MION								

5	ATOM	1891	CA	GLY A	120		34.655	-3.388	7.696	1.00 3	7.27			С
	ATOM	1894	C .	GLY A	120		34.278	-4.619	6.920	1.00 3	5.23			С
	ATOM	1895	0	GLY A	120		35.044	-5.538	6.888	1.00 4	1.95			0
	ATOM	1896	N	LEU A	121		33.116	-4.697	6.293	1.00 4	0.05			N
	MOTA	1898	CA	LEU A	121		32.866	-5.891	5.473	1.00 3	4.58			С
10	ATOM	1900	CB	LEU A	121		31.626	-6.622	5.917	1.00 3	5.45			C
	ATOM	1903	CG	LEU A	121		31.436	-6.831	7.393	1.00 3	1.35			С
	ATOM	1905	CD1	LEU A	121		29.950	-6.863	7.687	1.00 2	8.15			С
	ATOM	1909	CD2	LEU A	121		32.124	-8.105	7.719	1.00 2	8.77			С
	ATOM	1913	С	LEU A	121		32.704	-5.635	3.984	1.00 3	7.29			·C
15	ATOM	1914	0	LEU A	121	٠.	32.158	-6.483	3.267	1.00 4	2.02			0
	MOTA	1915	N	ALA A	122		33.145	-4.505	3.469	1.00 3	6.05			N
	ATOM	1917	CA	ALA A	122		33.084	-4.404	2.029	1.00 3	9.37			С
	ATOM	1919	CB	ALA A	122		32.974	-3.039	1.593	1.00 4	0.38	• .	•	. C
*	MOTA	1923	С	ALA A	122		34.289	-5.090	1.398	1.00 4	1.97			С
20	ATOM	1924	0	ALA A			35.020	-5.841	2.046	1.00 4	0.99			0
	ATOM	1925	N	TYR A	123		34.486	-4.796	0.124	1.00 4	3.02			N
	ATOM	1927	CA	TYR A	123		35.423	-5.522	-0.690	1.00 4	0.35			C
	MOTA	1929	CB	TYR A	123		34.904	-5.453	-2.091	1.00 3	8.74			C
	. ATOM	1932	CG	TYR A	123		33.687	-6.306	-2.361	1.00 4	1.64			C
25	ATOM	1933	CD1	TYR A	123		32.453	-5.755	-2.557	1.00 3	9.22			С
•	ATOM	1935	CE1	TYR A	123		31.352	-6.564	-2.824	1.00 3	4.66			С
	MOTA .	1937	CZ	TYR A	123		31.487	-7.899	-2.896	1.00 3	6.31			С
	MOTA	1938	OH	TYR A	123		30.392	-8.724	-3.167	1.00 4	3.22			0
	ATOM	1940	CE2	TYR A	123		32.711	-8.459	-2.706	1.00 4	3.43			. C
30	ATOM	1942	CD2	TYR A	123		33.788	-7.686	-2.443	1.00 4	3.16			С
	MOTA	1944	С	TYR A	123		36.758	-4.856	-0.586	1.00 4	3.96			С
	ATOM	1945	0	TYR A	123		36.831	-3.746	-0.094	1.00 4	3.08			0
	ATOM	1946	N	ALA A	124		37.810	~5.509	-1.063	1.00 4	6.53			N
	MOTA	1948	CA	ALA A	124		39.194	-5.021	-0.894	1.00 4	5.27			C
35 .	MOTA	1950	CB	ALA A	124		40.163	-6.124	-1.311	1.00 4	5.24		•	С
	MOTA	1954	С	ALA A	124		39.597	-3.728	-1.616	1.00 4	7.88	•		C
	ATOM	1955	0	ALA A	124		40.511	-2.999	-1.159	1.00 4	7.35			0
	MOTA	1956	N	GLU A			38.950	-3.438	-2.735	1.00 4	6.72			N
	MOTA	1958	CA	GLU A	125		39.399	-2.342	-3.574	1.00 4	6.92			С
40	MOTA	1960	CB	GLU A	125		38.461	-2.169	-4.774	1.00 4	9.10			C
	ATOM	1963	CG	GLU A	125		38.608	-0.831	-5.492	1.00 5				С
	MOTA	1966	CD	GLU A	125		37.786	-0.739	-6.766	1.00 5				С
	MOTA	1967		GLU A			37.095	-1.730	-7.135	1.00 5				0
	MOTA	1968		GLU A			37.819	0.355	-7.409	1.00 6				0
45	MOTA	1969	С	.GLU A			39.511	-1.074	-2.753	1.00 .4				С
	ATOM	1970	0	GLU A			40.486	-0.298	-2.858	1.00 5		•		0
	ATOM	1971	N	ILE A			38.521	-0.843	-1.908	1.00 4				N
	MOTA	1973	CA	ILE A			38.561		-1.157					С
	ATOM	1975	CB	ILE A			37.142	0.953	-0.961	1.00 4				, C
50	MOTA	1977		ILE A			36.254	0.022	-0.122	1.00 4				С
	MOTA	1980		ILE A			34.965	0.642	0.383	1.00 5				С
	MOTA	1984	CG2	ILE A	126		36.539	1.274	-2.351	1.00 4	6.90			С
	ATOM	1988	С	ILE A		: .	39.288	0,228	0.142	1.00 4	4.66			C.
	MOTA	1989	0	ILE A			39.146	1.085	1.007	1.00 4	8.22			0
55	ATOM.	1990	N	ALA .A		• •	40.093	-0.808		1.00 4	4.81	••		N
	MOTA	1992	CA	ALA A	127		40.788	-0.914	1.580	1.00 4				C
	· ATOM	1994	CB	ALA A			40.982	-2.321	1.937	1.00 5				С
	MOTA	1998	C	ALA A	127		42.119	-0.200	1.613	1.00 5		•		. C
	ATOM	1999	0	ALA A	127		42.699	0.145	0.574	1.00 5	9.40			0
60	ATOM	2000	·N	ARG A	128		42.591	0.010	2.838	1.00 5	1.36			N
	MOTA	2002	CA	ARG A	128		43.783	0.715	3.064	1.00 5	1.80			C.

			100		43.430	1.900	3.897	1.00 56.05		C	
5	MOTA	2004 CB	ARG A 128			2.626		1.00 59.64		(
•	MOTA	2007 CG	ARG A 128		42.275	2.934		1.00 69.11	•	(3
	MOTA	2010 CD	ARG A 128		42.295	4.108	1.663	1.00 79.76	•	1	N
	MOTA	2013 NE	ARG A 128		41.482			1.00 81.91		(2
	ATOM	2015 CZ	ARG A 128		41.839	5.318	2.630	1.00 80.28		1	N
10	MOTA		ARG A 128		43.001	5.508		1.00 87.99			N
	ATOM	2019 NH2	ARG A 128		41.039	6.335		1.00 51.97			С
	MOTA	2022 C	ARG A 128		44.831	-0.135		1.00 49.70			o
	ATOM	2023 O	ARG A 128		44.461	-0.987		1.00 44.07			N
	ATOM	2024 N	PRO A 129		46.129	0.076		1.00 44.07			c ·
15	ATOM	2025 CA		: .		1.004					c
13	ATOM	2027 CB	PRO A 129		48.105	0.812	•	1.00 39.26			
	MOTA	2030 CG	PRO A 129		48.386	-0.019		1.00 44.63			c
	ATOM	2033 CD	PRO A 129		47.196	-0.642		1.00 43.20			c
•		2036 C	PRO A 129		46.254	0.674	1.113	1.00 45.48			0
20	MOTA	2037 0	PRO A 129		46.153	1.658	0.336	1.00 46.05			
20	MOTA	2037 O	ASP A 130		46.101	-0.637	0.783	1.00 46.52			N
	ATOM		ASP A 130		45.574	-1.009	-0.520	1.00 47.07			C
	MOTA		ASP A 130		46.563		-1.653	1.00 52.49			C
	MOTA	2042 CB	ASP A 130		47.874	-1.365	-1.520	1.00 58.99			С
	MOTA	2045 CG	ASP A 130		48.849	-0.917	-2.187	1.00 66.76			0 ,
25	MOTA		2 ASP A 130		48.023		-0.794	1.00 64.97			0 -
	MOTA				44.937	-2.355	-0.652	1.00 44.59			С
	ATOM	2048 C	ASP A 130		44.877		0.272	1.00 50.22			0
:.	MOTA	2049 O	ASP A 130		44.443	-2.606	-1.834	1.00 41.96			N
	ATOM.	2050 N	ASP A 131		43.679		-2.024	1.00 45.38	•		С
30	MOTA	. 2052 CA	ASP A 131			-3.828	-3.427	1.00 45.37			C
	MOTA	2054 CB			43.076	-4.043	-4.476	1.00 54.14			С
	MOTA	2057 CG	ASP A 131		44.106		-4.143	1.00 60.53			0
•	MOTA		1 ASP A 131		45.130	-4.692 -3.593	-5.648	1.00 58.51			0
	ATOM		2 ASP A 131		43.983		-1.770	1.00 41.04			С
35	MOTA	2060 C	ASP A 131		44.437	-5.085	-2.065	1.00 49.55		•	0
	MOTA	2061 O	ASP A 131		43.912	-6.123		1.00 39.75			N
	MOTA	2062 N	SER A 132	•	45.645	-5.050	-1.247	1.00 45.06		٠.	С
	MOTA	2064 CA	SER A 132		46.409	-6.304	-1.002	1.00 43.25	•		С
	MOTA	2066 CE	SER A 132		47.788	-6.174	-1.605	1.00 43.23			Ō
40	ATOM	2069 00	SER A 132		48.375	-4.995	-1.060	1.00 33.72			Č
	MOTA	2071 C	SER A 132		46.582	-6.591	0.489	1.00 41.26			0
	MOTA	2072 0	SER A 132		47.588		0.938	1.00 52.36			N
	ATOM	2073 N	LEU A 133		45.584		1.242	1.00 43.42			C
	ATOM	2075 C	4.00		45.558		2.687	1.00 44.69			C
45	ATOM	2077 CI	400		45.773		3.419	1.00 41.73			č
43		2080 C			45.518	-5.228		1.00 41.79			c
	MOTA		D1 LEU A 133		46.832	-5.498	5.559	1.00 39.80			
	MOTA		D2 LEU A 133		44.771		5.716	1.00 44.00		•	Ç
	ATOM	_			44.166	-6.677	2.929	1.00 47.10			Ċ
	MOTA				43.330	-5.956	3.439	1.00 51.69			0
50		2091 0			43.977		2.510	1.00 51.73			N
	MOTA	2092 N			42.777		2.630				С
	ATOM	2094 C			42.77	-10.178	2.777	1.00 47.21			С
•	MOTA				43.441	-11.212	3.013				. C
	MOTA		G GLU A 134	٠	42.10	-12.623	2.755		•	٠.	C
55	MOTA		D GLU A 134		42.68	7 -12 074	1.569		-1.		Ö
	MOTA	2103 C	E1 GLU A 134		42.980	12.874					. 0
	ATOM	2104 C	E2 GLU A 134			7 -13.448					С
	MOTA		GLU A 134		41.83	7 -8.500				•	· o
	MOTA				42.23						N
- 60			PRO A 135		40.57					•	·C
	ATOM		A PRO A 135		39.53	1 -8.099	4.437	1.00 37.41			. •
		-						*			

5 .	ATOM	2110	CB	PRO	Α	135	38	. 355	-7.629	3.597	1.00	37.44			C
	MOTA	2113	CG	PRO	Α	135	38	.853	-7.363	2.237	1.00	40.45			C
	ATOM	2116	CD	PRO	Α	135	40	.071	-8.171	2.068	1.00	42.71			C
	ATOM	2119	С	PRO	Α	135	39	.174	-9.353	5.269	1.00	36.44			С
	MOTA	2120	0	PRO	Α	135	39	.366	-10.450	4.767	1.00	34.69			0
- 10	ATOM	2121	N	PHE	Α	136	38	. 668	-9.163	6.505	1.00	35.67			N
	ATOM	2123	.CA	PHE	Α	136	38	.233	-10.241	7.427	1.00	31.72			C
	ATOM	2125	CB	PHE			37	.463	-9.676	8.625	1.00	27.91			С
	ATOM	2128	CG	PHE					-10.727	9.517	1.00	28.87			С
	ATOM	2129		PHE					-11.301	10.550	1.00	32.96			· C
15	ATOM	2131		PHE					-12.267	11.382	1.00	33.11			С
	ATOM	2133	CZ	PHE					-12.663	11.195	1.00	33.91			С
	ATOM	2135		PHE					-12.111	10.175	1.00	36.07			С
	ATOM	2137		PHE					-11.137	9.333		37.92			C.
•	ATOM	2139		PHE					-11.218	6.753	1.00	35.77			С
20	ATOM	2140	Ö	PHE					-12.376	6.668		45.44	•		0
20	ATOM	2141	N	PHE					-10.778	6.261		40.56			N
	ATOM	2143	CA	PHE					-11.754	5.677		43.42			C.
	ATOM	2145	CB	PHE					-11.132	5.014		43.68			C
	ATOM	2148		PHE					-12.067	5.028		41.41			Ċ
25	ATOM	2149		PHE					-12.231	6.160		38.90			č
23	ATOM	2151		PHE					-13.107	6.179		36.47			Ċ
•	ATOM	2153	CZ	PHE					-13.824	5.087		36.88			č
	ATOM	2155		PHE					-13.682	3.958		39.68			č
		2157		PHE					-12.809	3.922		43.99			č
30	ATOM ATOM	2159		·PHE					-12.571	4.704		43.89			c
,50		2160	•	PHE					-13.774	4.828	•	41.80			o.
	ATOM		0				-		-11.904	3.762		47.91			N
	MOTA	2161	N	ASP					-12.581	2.776		47.51			C
	ATOM	2163	CA CB	ASP ASP					-11.632	2.142		51.24			ç
35	ATOM ATOM	2165 2168	CG.	ASP					-11.344	0.725		54.56			č
))	ATOM	2169		ASP					-12.027	-0.179	•	66.25		•	ō
	ATOM	2170		ASP					-10.434	0.419		57.65			ŏ
	ATOM	2171	C	ASP					-13.684	3.394	•	47.78			Č
	ATOM	2172	0	ASP		_			-14.788	2.886		57.75			ō
40	ATOM	2172	N	SER					-13.385	4.482		46.16			N
40	ATOM	2175	CA	SER					-14.405	5.145		42.31			Ċ
	ATOM	2177	CB			139			-13.740	6.204		42.45			Č
	ATOM	2180				139			-12.754	5.615		35.20			ő
	ATOM	2180	C			139			-15.421	5.797		43.01			č
45	ATOM	2183	0			139			-16.570	5.891		42.82			Ö
43	ATOM	2184	N			140			-15.016	6.279	•	50.41			N
•	ATOM	2186	CA	LEU					-15.973	7.006		46.59			c
	ATOM		CB.						-15.302			47.69			č
						140				8.248		54.03			Č
50	ATOM	2191	CG						-16.175	9.380		56.74			č
50	ATOM	2193		LEU					-16.828	8.755		52.27			c
	MOTA	2197		LEU					-15.327	6.139					c
	MOTA	2201	C			140			-17.129	6.649		48.27			o
	MOTA	2202		LEU					-18.231			48.66			
	MOTA	2203	N			141			-16.868	4.833		46.25	•		N
55	ATOM	2205		VAL					-17.909	3.873	••	48.65		•	C
	MOTA	2207	CB			141			-17.376	2.644		49.70			C
	ATOM	2209				141			-18.555	1.662		50.68			C
	MOTA	2213		VAL					-16.801	3.069		50.47			C
	MOTA	2217	С			141 .			-18.777	3.388		54.04			С
60	ATOM	2218	0			141			-19.989	3.354		62.33			0
	MOTA	2219	N	LYS	A	142	38	.390	-18.195	3.009	τ.00	53.50			N

			39.497 -18.997 2.510 1.00 51.72 C	
5	MOTA	2221 CA LYS A 142	10 720 10 173 2 027 1.00 51.19	
-	MOTA	2223 CB LYS A 142	10.466 -16.996 1.006 1.00 55.43	
	MOTA	2226 CG LYS A 142	41 700 -16 385 0.423 1.00 59.35	
	ATOM	2229 CD LYS A 142	41.737 -15.659 -0.919 1.00 61.18	
	MOTA	2232 CE LYS A 142	41.577 = 15 043 =0.953 1.00 69.14 N	
10	ATOM	2235 NZ LYS A 142	20.070 -20.002 3.571 1.00 52.97 C	
10	ATOM	2239 C LYS A 142	39.970 20.002 3.211 1.00 55.66	
	ATOM	2240 O LYS A 142	40.643 -20.500 4.851 1.00 47.49 N	
	ATOM	2241 N GLN A 143	39.634 10.630 5 937 1 00 47.98 C	
	ATOM	2243 CA GLN A 143	40.103 20 777 7 058 1 00 44.95 C	
15	ATOM	2245 CB GLN A 143	40.818 -13.17 40.100 10.165 6.780 1.00 45.74 C	
13	ATOM	2248 CG GLN A 143	42.100 13.100	
	MOTA	2251 CD GLN A 143	42.322 1	
	ATOM	2252 OE1 GLN A 143	42.546 16.703 7.081 1.00 48.24 N	
•	ATOM	2253 NE2 GLN A 143	44.101 1000	
20	ATOM	2256 C GLN A 143	39.190 21.30	
20	MOTA	2257 O GLN A 143	39.JUJ 22.22	
	MOTA	2258 N THR A 144	31.303 21.0.0	
	MOTA	2260 CA THR A 144	30.313 22	
		2262 CB THR A 144	30.223 21.73	
25	MOTA	2264 OG1 THR A 144	35.191 -20.904 7.267 1.00 50.10	
25	MOTA	2266 CG2 THR A 144	37.139 -20.769 8.490 1.00 53.55	
	MOTA	2270 C THR A 144	35.875 -22.756 5.581 1.00 55.57	
:	MOTA	2271 O THR A 144	36.071 -22.385 4.425 1.00 51.12 N	
	MOTA	2272 N HIS A 145	34.772 -23.401 5.946 1.00 37.36	
20	ATOM	2274 CA HIS A 145	33.786 -23.769 4.930 1.00 61.40	
30	ATOM	2276 CB HIS A 145	33.315 -25.229 5.146 1.00 00.00	
	ATOM	2279 CG HIS A 145	34.393 -26.252 4.917 1.00 73.31 N	
	MOTA	2280 ND1 HIS A 145	35.092 -26.844 5.950 1.00 75.22	
	MOTA		35.980 -27.687 5.453 1.00 77.07	
	MOTA	2282 CE1 HIS A 145 2284 NE2 HIS A 145	35.882 -27.665 4.134 1.00 75.10	
. 35	MOTA	145	34.897 -26.777 3.774 1.00 73.10 C	
	MOTA	C NTC 7 1/5	32.587 -22.826 4.899 1.00 57.36	
	MOTA		31.592 -23.086 4.214 1.00 57.76	
	MOTA	146	32.679 -21.728 5.629 1.00 52.17	
	MOTA	1 146	31.539 -20.847 5.769 1.00 47.04	
. 40	MOTA	**** * 146	31.849 -19.669 6.681 1.00 48.57	
	MOTA	COL WAT A 146	30.713 -18.715 6.687 1.00 46.07	
•	ATOM	1 1 A C	32.122 -20.147 8.110 1.00 49.76 C	
	ATOM		31.247 -20.301 4.426 1.00 42.53	
	MOTA	230.	32 116 -19.728 3.817 1.00 45.79	
45		· 11 DDO 7 147	30.029 -20.472 3.950 1.00 37.44	
	ATOM	2227 CN DDO A 147	29 613 -19.931 2.649 1.00 36.26	
	MOTA	on DDO 7 147	20:130 -20 275 2.599 1:00 30:01	
	ATOM	co ppo 7 147	28 062 -21.485 3.451 1.00 37.97	
	MOTA	7 147	28 953 -21.213 4.609 1.00 37.03	
50	OTA:	2315 CD PRO A 147	20 703 -18 397 2.535 1.00, 38.02	
	ATO!	2318 C PRO A 147	29 688 -17 668 3.519 1.00 36.50	
	ATO		30_042 -17.926 1.318 1.00 37.03	
	. ATO	M 2320 N ASN A 148	30 370 -16.536 1.041 1.00 35.69	
	OTA	M 2322 CA ASN A 148	31 113 -16 480 -0.280 1.00 35.18	
5.		M 2324 CB ASN A 148	31.791 -15.208 -0.460 1.00 38.29	
	ATO	M 2327 CG ASN A 148	31 990 -14 492 0.507 1.00 48.87	
	ATO	M 2328 OD1 ASN A 148	31.990 14.990 -1 683 1.00 45.21	
	OTA	M 2329 ND2 ASN A 148	32.170 11.500 0.950 1.00 37.44	
	ATO	M 2332 C ASN A 148	29.104 15.501 -0.110 1.00 34.38	
. 6		M 2333 O ASN A 148	20.320 11.33	N
J	ATC	17 TEN 10 149	28.498 -15.407 2.075 1.00 39.14	

	•	5 140	27.269 -14.634 2.168 1.00 37.49 C
5	MOTA	2336 CA LEU A 149	06 071 -15 476 1 699 1.00 38.02 C
	MOTA.	2338 CB LEU A 149	24.571 15 300 2 049 1.00 45.01 C
	MOTA	2341 CG LEU A 149	27.042 -16 146 1 018 1.00 46.47 C
	MOTA	2343 CD1 LEU A 149	23.043 25.749 3.449 1.00 46.97 C
	MOTA	2347 CD2 LEU A 149	07 073 14 349 3 619 1.00 41.29 C
10	MOTA	2351 C LEU A 149	27.073 =14.349
•	ATOM	2352 O LEU A 149	oc 507 12 160 3 957 1.00 43.88 N
	MOTA	2353 N PHE A 150	26.597 -13.160 3.957 1.00 43.88 26.128 -12.896 5.313 1.00 37.90 C
	MOTA	2355 CA PHE A 150.	27.151 12.169 6.146 1.00.36.97 C
	MOTA	2357 CB PHE A 150	57 514 10 955 5 616 1 00 38 62 C
15	ATOM	2360 CG PHE A 150	C 10 721 4 664 1 00 43 40
_	MOTA	2361 CD1 PHE A 150	28.508 =10.751 4.003
	MOTA	2363 CE1 PHE A 150	28.849 -9.516 4.157 1.00 36.52 28.202 -8.415 4.609 1.00 39.56
	MOTA	2365 CZ PHE A 150	28.202 -8.415 4.005 1.00 32 53 C
•	ATOM	2367 CE2 PHE A 150	27.220 -8.330 3.304 1.00 3.6
20	ATOM	2369 CD2 PHE A 150	26.885 -9.737 0.033 1.00 3
20	MOTA	2371 C PHE A 150	24.854 -12.097 5.122 1.00
٠.	ATOM	2372 O PHE A 150	24.632 -11.537 4.054 1.00 12.00
	ATOM	2373 N SER A 151	23.980 -12.0/1 0.121 1.00
	ATOM	2375 CA SER A 151	22.760 -11.287 0.010 1.00
25	ATOM	2377 CB SER A 151	21.553 -12.207 5.931 1.00 45.00
2.5	ATOM	2380 OG SER A 151	21.6/3 -13.313 0.803 1.00 33
	ATOM	2382 C SER A 151	22.708 -10.401 7.238 1.30
	MOTA	2383 O SER A 151	23.371 -10.749 8.190 1.00 40.13
•	MOTA	2384 N LEU A 152	21.985 -9.260 7.214
30	MOTA	2386 CA LEU A 152	21.755 -8.446 0.455 1.00 25 00
50	ATOM	2388 CB LEU A 152	22.588 -7.166 6.446 1.66 60 60
	MOTA	2391 CG LEU A 152	24.121 -7.237 8.403 1.00 23.56
	ATOM	2393 CD1 LEU A 152	24.769 -5.957 8.014 1.00 20 11
	ATOM	2397 CD2 LEU A 152	24.536 -7.467 9.612 1.66 50.56
35	MOTA	2401 C LEU A 152	20.305 -8.042 8.672 1.00 3.0
22	MOTA	2402 O LEU A 152	19.591 -7.681 7.750 1.00 1.00
	ATOM	2403 N GLN A 153	19.877 -8.069 9.923 1.00 27.21
	MOTA	2405 CA GLN A 153	18.544 -7.609 10.332 1.00 3.00
	ATOM	2407 CB GLN A 153	17.636 -8.817 10.713 1.00 20 07
40	•ATOM	2410 CG GLN A 153	16.211 -8.476 11.173 1.00 17.20
+∪.	MOTA	2413 CD GLN A 153	15.562 -9.519 12.103
	ATOM	2414 OE1 GLN A 153	16.047 -9.755 13.231 1.00 30.00
	ATOM	2415 NE2 GLN A 153	14.465 -10.125 11.663 1.66 33.67
	ATOM	2418 C GLN A 153	18.798 -6.669 11.552 1.60 47 11
45	MOTA	2419 O GLN A 153	18.980 -7.157 12.636 1.00 17.15
73	ATOM	2420 N LEU A 154	18.830 -5.384 11.320 1.00 42.01
,	MOTA	2422 CA LEU A 154	19.057 -4.410 12.537 1.00 42.53
	ATOM	2424 CB LEU A 154	19.826 -3.221 11.035 1.00
	MOTA	2427 CG LEU A 154	21.012 -3.514 10.51.
50		2429 CD1 LEU A 154	21.452 -2.255 10.255
20	ATOM	2433 CD2 LEU A 154	22.13/ -4.06/ 11.735 1.35
•	MOTA	1 C /	17.700 -3.937 12.912 1.00 42.07
	MOTA		16.804 =3.804 12.130 2.00 30.1=
	ATOM	7 7 5 5	17.538 -3.646 14.191 1.00 45.97
55		aug 3 166	16.180 -3.612 14.763 1.00 51.90 C
55		CVG N 155	15.927 -4.865 15.662 1.00 51.86
	ATOM	ava 3 165	15.554 -6.528 14.975 1.00 51.81
	MOTA	155	15.967 -2.390 15.642 1.00 57.62
	MOTA	010 3 155	16.114 -2.476 16.878 1.00 63.11
-	ATOM		15.631 -1.257 15.041 1.00 58.85
60		OTY N 156	15.380 -0.072 15.830 1.00 62.65 C
	ATOM	I SAUT OU OUT " TOO	

											_
5	MOTA	2454	С	GLY A 156		14.226	-0.446	16.728	1.00 66.48		C
		2455	0	GLY A 156		13,447	-1.309	16.342	1.00 69.64		0
	ATOM	2456	N	ALA A 157		14.088	0.144		1.00 69.44		N
	ATOM	2458	ÇA	ALA A 157		12.896	-0.169	18.704	1.00 72.46		C
	ATOM	2460	CB	ALA A 157		13.304	-0.588	20.111	1.00 75.06		C
10	ATOM	2464	С	ALA A 157		11.799	0.960	18.698	1.00 73.42		С
	ATOM	2465	0 -	ALA A 157		10.749	0.888	19.359	1.00 73.68		0
	ATOM	2466	N	GLY A 158		12.015	2.000	17.926	1.00 74.47		N
	ATOM	2468	CA	GLY A 158		11.010	3.043	17.837	1.00 78.58		С
	ATOM.	2471	C	GLY A 158		10.829	3.954	19.059	1.00 82.73		С
15 ·	ATOM	2472	ō	GLY A .158		9.947	4.825	19.033	1.00 85.96		0
13	ATOM	2473	N	PHE A 159		11.633	3.774	20.115	1.00 83.55		N
	ATOM	2475	CA	PHE A 159		11.564	4.626	21.313	1.00 85.05	•	С
	MOTA	2477	CB	PHE A 159		10.558	4.054	22.277	1.00 85.74		С
•	MOTA	2480	CG	PHE A 159		10.993	2.748	22.855	1.00 82.94		C .
20	ATOM	2481		PHE A 159		10.305	1.593	22.561	1.00 82.82		С
20	ATOM	2483		PHE A 159		10.717	0.373	23.096	1.00 83.66		С
	ATOM	2485	CZ	PHE A 159		11.831	0.325	23.935	1.00 82.59		С
	ATOM	2487		PHE A 159		12.519	1.491	24.228	1.00 80.31		C
	MOTA	2489		PHE A 159		12.099	2.683	23.686	1.00 79.87		С
25	ATOM	2491		PHE A 159		12.910	4.671	22.044	1.00 87.61	•	C
25		2491	0	PHE A 159		13.494	3.624	22.302	1.00 87.56		0
	ATOM	2492	N -	PRO A 160		13.383	5.862	22.418	1.00 89.61		N
	MOTA	2493	CA	PRO A 160		14.743		22.954	1.00 91.86		С
•	MOTA		CB	PRO A 160		14.714	7.423	23.610	1.00 92.67		,C
20	ATOM	2496	. CG	PRO A 160			8.102	23.127	1.00 90.33		Ċ
30	ATOM	2499 2502	CD	PRO A 160		12.656	7.139	22.372	1.00 90.15		С
	MOTA	2502	С	PRO A 160		15.261	5.019	23.970	1.00 91.59		С
	MOTA	2505		PRO A 160		14.535	4.311	24.654	1.00 87.47		0
	ATOM		N.	LEU A 161		16.582	5.002	24.046	1.00 94.49		N
35	MOTA	2507	CA	LEU A 161		17.318	4.103	24.906	1.00 97.03		С
33	MOTA	2509 2511	CB	LEU A 161		17.885	2.918	24.078			С
	ATOM	2514	CG	LEU A 161		17.017	1.707	23.671	1.00 94.82		С
	ATOM	2514		LEU A 161		17.658	0.923	22.493	1.00 93.82	•	С
	ATOM	2520		LEU A 161		16.735	0.783	24.864	1.00 93.08		С
40	ATOM	2524	C	LEU A 161		18.475	4.906	25.503	1.00 98.82		С
40	ATOM	2525	Ö	LEU A 161		18.848	5.967	24.987	1.00 98.25		0
	ATOM	2526	N	GLN A 162		19.013	4.404	26.608	1.00101.00		N
	MOTA		CA	GLN A 162		20.290		27.135	1.00101.95		С
	MOTA	2528		GLN A 162		20.225			1.00103.13		С
15	MOTA	2530	CG	GLN A 162		19.060	. 5:934	29.201	1.00102.96		С
45	MOTA	2533	CD	GLN A 162		18.651	5.522	30.624	1.00104.66		С
	ATOM	2536		L GLN A 162		17.703	6.076	31.190	1.00104.03		0
٠.	ATOM	2537		2 GLN A 162		19.365			1:00103.68		· N
	ATOM	2538				21.315	3.748	26.850	1.00102.26		С
	ATOM	2541	C.	GLN A 162		20.958	2.612	26.522			0
50	ATOM	2542	0.	GLN A 162		22.593		26.965	1.00104.53		N
	ATOM	2543	N	GLN A 163			3.073	26.995	1.00105.21	•	С
	ATOM	2545	CA	GLN A 163		23.655			1.00105.72		C
	MOTA	2547			•	24.906	3.716	27.928	1.00105.72		Ċ
	ATOM	2550	CG	GLN A 163		26.028	2.741		1.00103.40		C
55	MOTA	2553		GLN A 163		27.384	3.435	27.930 28.924	1.00103.07		Ò.
	MOTA	2554		1 GLN A 163		27.767	4.048				N
	MOTA	2555		2 GLN A 163		28.105		26.814	1.00101.46		C
	MOTA	2558	С	GLN A 163		23.314		27.894	1.00105.84		0
	MOTA	2559	0	GLN A 163		23.625			1.00105.65		N
60	MOTA	2560		SER A 164		22.684			1.00105.53		C
	MOTA	2562	CA	SER A 164		22.315	1.146	30.020	1.00105.77		Ç

5	ATOM	2564	СВ	SER	A 164		21.632	1.798	31.227	1.00106.94	•		С
•	ATOM	2567	OG	SER .	A 164		21.798	1.017	32.400	1.00107.14			0
	ATOM	2569	С	SER .	A 164		21.335	0.192	29.374	1.00105.64	-		С
	MOTA	2570	0	SER .	A 164		21.407	-1.065	29.492	1.00105.75			0
	ATOM	2571	N	GLU .	A 165		20.403	0.835	28.682	1.00102.30			N
10	ATOM	2573	CA	GLU .	A 165		19.381	0.105	27.976	1.00 98.16			С
	MOTA	2575	CB	GLU .	A 165		18.355	1.082	27.415	1.00 98.15	•		С
	ATOM	2578	CG	GLU .	A 165		17.997	2.126	28.479	1.00 99.91			С
	ATOM	2581	CD	GLU .	A 165		16.584	2.687	28.403	1.00 98.66			С
	MOTA	2582	OE1	GLU .	A 165		15.621	1.933	28.642	1.00 94.69			O
15	ATOM	2583	OE2	GLU	A 165		16.444	3.900	28.123	1.00100.25			0
	ATOM	2584	С	GLU	A 165		20.072	-0.690	26.891	1.00 95.52			С
	ATOM	2585	0	GLU .	A 165		19.903	-1.909	26.807	1.00 92.32			, О
	ATOM	2586	N	VAL	A 166		20.884	0.002	26.095	1.00 92.23			N
•	ATOM	2588	CA	VAL	A 166		21.552	-0.618	24.959	1.00 90.08			С
20	ATOM	2590	CB	VAL	A 166		22.637	0.280	24.385	1.00 89.46			С
	ATOM	2592	CG1	VAL	A 166		23.997	-0.471	24.238	1.00 89.54			С
	ATOM	2596			A 166		22.180	0.834	23.067	1.00 89.64			С
	ATOM	2600	С		A 166	-	22.155	-1.969	25.275	1.00 89.54			С
	ATOM	2601	0	VAL	A 166	:	21.868	-2.949	24.587	1.00 90.45			0
25	ATOM	2602	N	LEU	A 167		22.988	-2.039	26.306	1.00 89.05			N
	ATOM	2604	CA		A 167		23.644	-3.308	26.620	1.00 88.10			С
	ATOM	2606	CB		A 167.		24.572	-3.201	27.852	1.00 87.51			С
	ATOM	2609	СĠ	LEU	A 167		25.665	-2.130	27.780	1.00 89.06	•		С
	ATOM	2611	CD1	LEU	A 167.		25.990	-1.526	29.151	1.00 88.01		•	С
30	ATOM	2615	CD2	LEU	A 167		26.921	-2.670	27.122	1.00 88.50			С
- :	ATOM	2619	С	LEU	A 167		22.606	-4.403	26.851	1.00 84.50			С
	ATOM	2620	0	LEU	A 167		22.770	-5.521	26.386	1.00 82.46			0
•	MOTA	2621	N ·	ALA	A 168		21.533	-4.071	27.554				N
	ATOM	2623	CA	ALA	A 168		20.565	-5.083	27.974	1.00 83.99			C
35	ATOM	2625	CB ·	ALA	A 168		19.807	-4.567	29.200	1.00 84.06			С
	ATOM	2629	С	ALA	A 168		19.560	-5.604	26.929	1.00 84.00	•		С
	ATOM	2630	0	ALA	A 168		18.918	-6.627	27.179	1.00 83.07			0
	ATOM	2631	N	SER	A 169		19.423	-4.940	25 .7 76	1.00 82.75	•		N
	MOTA	2633	CA	SER	A 169		18.339	-5.295	24.845	1.00 82.41			С
40	MOTA	2635	CB	SER	A 169		17.199	-4.258	24.968	1.00 83.85			Ç
	ATOM	2638	OG	SER	A 169		16.810	-4.032	26.327	1.00 80.23		٠.	0
	ATOM	2640	·C	SER	A 169		18.735	-5.521	23.349	1.00 81.77			C
	MOTA	2641	0	SER	A 169		19.377	-4.675	22.718	1.00 80.20			0
	ATOM	2642	N	VAL	A 170		18.303	-6.674	22.816	1.00 79.25			N
45	MOTA	2644	CA		A 170		18.634	-7.170	21.469	1.00 74.78			С
	MOTA	2646	CB		A 170		17.885	-8.506	21.198	1.00 76.32			C
	MOTA	2648			A 170		18.278	-9.111	19.831	1.00 75.02			C
	ATOM	2652	CG2		A 170		18.143			1.00 77.47			C
	ATOM	2656	С		A 170		18.329	-6.185	20.326	1.00 70.08			C
50	MOTA	2657	0	VAL	A 170		17.197	-5.720	20.160	1.00 70.47			0
	MOTA	2658	N		A 171		19.345	-5.895	19.525	1.00 58.93			N
	MOŢA	2660	CA	GLY	A 171		19.208	-4.921	18.482	1.00 51.34			C
•	ATOM	2663	C	GLY	A 171		19.305	-5.525	17.115	1.00 47.82			С
	ATOM	2664	0	GLY	A 171		19.166	-4.812	16.149				0
55	ATOM	2665	N		A 172		19.548	-6.821	16.992				N
	ATOM	2667	CA	GLY	A 172		19.604	-7 . _, 381	15.654	1.00 40.82		•	С
	MOTA	2670	С		A 172		20.369	-8.678	15.473	1.00 42.31			C
	. ATOM .	2671	0	GLY	A 172	٠	20.653		16.439	1.00 39.19			0
	MOTA	2672	N		A 173		20.705			1.00 39.65			N
60	MOTA	2674	CA		A 173			-10.233	13.857	1.00 37.97			C
	ATOM	2676	CB	SER	A 173		20.194	-11.203	13.497	1.00 36.33			С

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1.00 46.54
                       SER A 173
                                       19.416 -11.435
                                                       14.634
            2679
                  OG
     MOTA
                                                                1.00 39.01
                                                        12.664
                                       22.205 -10.181
     ATOM
            2681
                  С
                       SER A 173
                                                                1.00 36.11
                                                                                       0
                                       21.805 -9.673
                                                        11.590
                       SER A 173
     MOTA
            2682
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                                                        12.853
                                                                                       N
                       MET A 174
                                       23.411 -10.705
                                                                1.00 35.19
     MOTA
            2683
                  N
                                                                 1.00 40.44
                       MET A 174
                                       24.339 -10.883
                                                        11.749
            2685
                  CA
     ATOM
                                                                1.00 40.55
                                                        12.040
                       MET A 174
                                       25.676 -10.261
10
     ATOM
            2687
                  CB
                                                                1.00 45.60
                       MET A 174
                                       26.481 -10.176
                                                        10.760
            2690
                  CG
     ATOM
                                       28.136 -9.627
                                                                1.00 47.63
                                                        10.960
     MOTA
            2693
                   SD
                       MET A 174
                                                                                       С
                                                                1.00 54.56
                                       28.387 -10.094
                                                        12.700
     MOTA
            2694
                   CE
                       MET A 174
                                       24.483 -12.394
                                                                 1.00 41.84
                                                                                       С
                       MET A 174
                                                        11.516
     MOTA
            2698
                  С
                                       25.013 -13.111
                                                                                       O
                       MET A 174
                                                        12.356
                                                                 1.00 48.31
15
     ATOM
            2699
                   0
                                                                 1.00 38.41
                                                                                       N
                       ILE A 175
                                       24.003 -12.875
                                                        10.383
            2700
     MOTA
                   N
                                                                                       C
                                                                1.00 37.39
                                       23.939 -14.288
                                                        10.136
                       ILE A 175
     ATOM
            2702
                   CA
                                                                1.00 39.69
                                                                                       С
                       ILE A 175
                                       22.628 -14.676
                                                         9.443
            2704
                   CB
     MOTA
                                                                1.00 40.97
                                       21.448 -14.387
                                                        10.364
            2706
                   CG1 ILE A 175
     MOTA
                                                                1.00 36.79
                                                        11.578
                                       21.449 -15.213
            2709
                   CD1 ILE A 175
20
     ATOM
                                                                1.00 35.35
                                                                                       C
                                       22.653 -16.089
                                                         9.035
                   CG2 ILE A 175
     MOTA
            2713
                                                                                       C
                       ILE A 175
                                       25.021 -14.522
                                                         9.202
                                                                 1.00 38.73
     ATOM
            2717
                   С
                                                                 1.00 40.30
                                                                                       0
                                       24.892 -14.246
                                                         8.037
                   0
                       ILE A 175
            2718
     ATOM
                                                                 1.00 42.09
                                                                                       N
                                       26.109 -15.038
                                                         9.722
                       ILE A 176
     ATOM
            2719
                   N
                                                                 1.00 37.74
                                                                                       C
                       ILE A 176
                                                         8.926
25
            2721
                   CA
                                       27.257 -15.301
     ATOM
                                                                                       C
                                                                 1.00 35.36
                                       28:382 -15.377
                                                         9.844
     MOTA
            2723
                   CB
                       ILE A 176
                                       28.371 -14.125
                                                        10.699
                                                                 1.00 32.86
                   CG1
                       ILE A 176
     ATOM
             2725
                                                                                       С
                                                                1.00 37.77
                                       29.740 -13.602
                                                        11.051
                       ILE A 176
     ATOM
             2728
                   CD1
                                                                                       C
                                       29.673 -15.621
                                                         9.060
                                                                 1.00 38.65
                   CG2 ILE A 176
     MOTA
             2732
                                                                                       С
                                       27.119 -16.617
                                                         8.202
                                                                 1.00 43.85
                   C
                       ILE A 176
            2736
     ATOM .
                                                                                       0
                                                                 1.00 49.67
                       ILE A 176
                                       27.178 -17.681
                                                         8.802
     MOTA
             2737
                   O
                                       26.890 -16.568
                                                         6.912
                                                                 1.00 44.93
                                                                                       N
     ATOM
             2738
                   N
                       GLY A 177
                                                                                       C
                                                         6.139
                                                                 1.00 45.46
                                       27.003 -17.783
             2740
                       GLY A 177
     ATOM .
                   CA
                                                                 1.00 42.70
                                                                                       C
                                       25.734 -18.428
                                                         5.673
                       GLY A 177
     ATOM
             2743
                   С
                                                         5.054
                                                                 1.00 47.24
                                                                                       Ŏ
                       GLY A 177
                                       25.751 -19.498
35
             2744
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     MOTA
                                                                1.00 40.94
                                                                                       N
                   N
                       GLY A 178
                                       24.619 -17.791
                                                         5.934
             2745
     ATOM
                                                                 1.00 38.84
                                                                                       С
                       GLY A 178
                                       23.369 -18.400
                                                         5.553
     ATOM
             2747
                   CA
                                                         5.705
                                                                 1.00 36.04
                                       22.355 -17.317
     ATOM
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                       GLY A 178
                                                         6.066
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                                                                                       N
                                       21.086 -17.636
                                                         5.418
40
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             2752
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                                       19.922 -16.748
                                                         5.502
                                                                 1.00 36.73
                       ILE A 179
     MOTA
             2754
                   CA
                                       19.262 -16.733
                                                          4.137
                                                                 1.00 38.18
                       ILE A 179
             2756
                   CB
     MOTA
                                                                                       C
                                                                 1.00 38.79
                   CG1 ILE A 179
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                                       15.272 -18.105
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                        HIS A 181
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             2787
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                        HIS A 181
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                   CE1 HIS A 181
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· 5	MOTA	2795	NE2	HIS A	181	٠	15.065	-20.328	3.950	1.00 79.2	27			N
	ATOM-	2797	CD2	HIS A	181		14.890	-20.439	5.310	1.00 71.5	55			С
	ATOM	2799	С	HIS A	181		12.983	-17.340	8.538	1.00 37.1		••		C
	ATOM	2800	0	HIS A				-16.873	8.232	1.00 39.5				ŏ
	ATOM	2801	N	SER A				-17.329	9.773	1.00 37.6				N
10		2803		SER A										
10	MOTA		CA.					-16.703	10.793	1.00 41.5				C
	ATOM	2805	CB	SER A				-17.234	12.149	1.00 42.1				С
•	MOTA	2808	OG	SER A				-16.913	12.339	1.00 43.8	39			0
	ATOM	2810	C	SER A			12.765	-15.204	10.848	1.00 39.2	23			С
	MOTA	2811	. 0	SER A	182		12:013	-14.548	11.554	1.00 46.7	71			0
15	ATOM	2812	· N	LEU A	183		13.730	-14.644	10.130	1.00 38.9	97			N
	ATOM	2814	CA	LEU A			13.967	-13.201	10.197	1.00 35.6				С
	ATOM		. CB	LEU A				-12.924	10.189	1.00 33.3				Č
	ATOM	2819	CG	LEU A		•		-13.474	11.374	1.00 31.8				Ç
20	ATOM	2821		LEU A				-13.477	11.088	1.00 31.7				С
20	MOTA	2825		LEU A				-12.666	12.607	1.00 41.8				С
	MOTA	2829	С	LEU A			13.318	-12.400	9.068	1.00 38.0)7			С
	ATOM	2830	0	LEU A			13.701	-11.288	8.820	1.00 42.0)4			0
	ATOM	2831	N	TYR A	184		12.336	-12.956	8.367	1.00 44.4	13			N.
	ATOM	2833	CA	TYR A	184		11.639	-12.209	7.320	1.00 33.3	34			Ċ
25	MOTA	. 2835	CB	TYR A				-12.087	6.063	1.00 38.7			•	C
	ATOM	2838	CG	TYR A				-13.281	5.134	1.00 35.8				č
	ATOM	2839		TYR A				-14.047	5.248	1.00 43.7				ċ
	ATOM	2841		TYR A										
-					•			-15.099	4.406	1.00 39.7				C
20	MOTA	2843	CZ	TYR A				-15.400	3.426	1.00 40.9				. C -
30	MOTA	2844	OH	TYR A				-16.460	2.577	1.00 45.5	55			0
	MOTA	2846		TYR A			12.159	-14.656	3.277	1.00 38.7	12			С
	ATOM	2848	CD2	TYR A	184		11.911	-13.599	4.127	1.00 36.4	17			C.
	ATOM	2850	C.	TYR A	184		10.304	-12.811	7.005	1.00 36.3	١6			С
	MOTA	2851	0	TYR A	184			-13.961	.7.352	1.00 30.8				0
35	ATOM	2852	N	THR A	•			-12.023	6.383	1.00 37.9				N
	ATOM	2854	CA	THR A				-12.549	5.846	1.00 40.8				c
	ATOM	2856	СВ	THR A				-11.913	6.441	1.00 43.1				c
	ATOM	2858		THR A				-10.491						
									6.207	1.00 43.9				0
40	MOTA	2860		THR A				-12.140	7.970	1.00 42.4				С
40	MOTA	2864	С	THR A				-12.271	4.378	1.00 37.6				С
	MOTA	2865	0	THR A				-11.408	3.929	1.00 36.3				O٠
	ATOM	2866	N	GLY A			-7.321	-12.992	3.637	1.00 34.8	36			N
	MOTA	2868	CA	GLY A	186		7.221	-12.791	2.205	1.00 37.3	11			С
	ATOM	2871	С	GLY A	186		8.449	-13.300	1.469	1.00 38.6	59			С
45	ATOM	2872	0	GLY A	186		9.179	-14.161	1.954	1.00 44.0)4			0
	ATOM	2873	N	SER A				-12.736	0.288	1.00 41.4				N
	ATOM	2875	CA	SER A				-13.062	-0.552	1.00 43.1			•	c
•	ATOM	2877						-13.063					•	
	ATOM	2880	OG	SER A				-13.003						Ċ
50									-2.139	1.00 54.9				0
50	ATOM	2882	С	SER A				-12.059	-0.443	1.00 44.8				С
	MOTA	2883	0	SER A				-10.938	0.064	1.00 42.3			٠.	0
	MOTA	2884	N	LEU A			12.094	-12.514	-0.943	1.00 39.2				N
	MOTA	2886	CA	LEU A	188	_	13.369	-11.810	-1.031	1.00 33.6	56			С
	ATOM	2888	CB .	LEU A	188	•	14.482	-12.824	-0.789	1.00 28.6				. C
55	ATOM	2891	CG	LEU A				-12.884	0.614	1.00 36.4				Ċ
	ATOM	2893		LEU A		•		-14.211	0.813	1.00 40.8				· Č
	ATOM	2897		LEU A				-11.777	0.889	1.00 34.4				C
	ATOM	2901	C	LEU A				-11.417	-2.474					
•	ATOM	2902								1.00 31.5				C
60			0	LEU A				-12.268	-3.294	1.00 41.6		•		0
UU	MOTA	2903	N.	TRP A				-10.177	-2.822	1.00 31.3				N
	ATOM	2905	CA	TRP A	189		14.040	-9.830	-4.230	1.00 33.7	70			С
							•							

				. 12 122	-8.688	-4.683	1.00 39.33		С
5	MOTA	2907 CB		13.132	-9.074	-4.947	1.00 37.95		C
	MOTA	2910 CG		11.729			1.00 35.87		C
	ATOM		1 TRP A 189	10.779	-9.313	-4.033	1.00 33.07		. N
	MOTA		1 TRP A 189	9.600	-9.646	-4.649			Ċ
	ATOM	2915 CE	2 TRP A 189	9.790	-9.626	-6.001	1.00 38.81		Ċ
10	ATOM	2916 CD	2 TRP A 189	11.125	-9.267	-6.224	1.00 35.31		
10	ATOM		3 TRP A 189	11.586	-9.181	-7.539	1.00 35.10		C
			3 TRP A 189	10.725	-9.447	-8.559	1.00 43.54		C
	MOTA		2 TRP A 189	9.384	-9.805	-8.305	1.00 44.03		. C
	MOTA		2 TRP A 189	8.904	-9.898	-7.034	1.00 40.92		С
	ATOM			15.493		-4.344	1.00 34.18		С
15	MOTA	2925 C	TRP A 189	15.950	-8.570	-3.567	1.00 34.73		Ο.
	MOTA	2926 O	TRP A 189			-5.317	1.00 34.76		N
	ATOM	2927 N	TYR A 190	16.217	-9.852	-5.412	1.00 36.58		С
	MOTA	2929 CA		17.603	-9.539		1.00 38.76		· c·
•	MOTA	2931 CE		18.341	-10.800	-5.769			č
20	ATOM	-2934 CG	TYR A 190		-11.826	-4.657	1.00 40.52		c
	ATOM		1 TYR A 190		-12.875	-4.609	1.00 43.16		
	MOTA	2937 CE		17.541	-13.817	-3.580	1.00 43.91	:	C
•	ATOM	2939 CZ		18.506	-13.685	-2.615	1.00 42.77		С
		2940 OF			-14.594	-1.566	1.00 46.77		0
00	ATOM		2 TYR A 190		-12.642	-2.677	1.00 35.63		С
25	ATOM				-11.742	-3.668	1.00 35.67		С
	MOTA			17.886	-8.451	-6.430	1.00 38.30		C
	MOTA	2946 C	TYR A 190	17.248	-8.420	-7.424	1.00 34.41		0
	ATOM	2947 O			-7.567	-6.133	1.00 41.18		N
	ATOM ·	2948 N		18.850		-7.025	1.00 37.26		С
30	MOTA	2950 C		19.299	-6.512		1.00 37.20		Ċ
	MOTA	2952 CI	B THR A 191	19.056	-5.091	-6.438	1.00 38.23		ŏ
	ATOM	2954 0	G1 THR A 191	19.283	-4.111	-7.448		•	Č
•	ATOM		G2 THR A 191	20.057		-5.419	1.00 31.07		C.
	ATOM	2960 C	THR A 191	20.782	-6.721	-7.200	1.00 39.94		
35	ATOM	2961 0		21.489	-7.008		1.00 41.73		0
. 55	. ATOM	2962 N		21.281	-6.578	-8.395	1.00 39.23		N
		2963 C		22.679	-6.840	-8.617	1.00 39.19		C
	MOTA	2965 C		22.824	-6.565	-10.111	1.00 41.47		С
	MOTA		G PRO A 192	21.484	~6.730	-10.671	1.00 36.70		С
46	MOTA		D PRO A 192	20.603			1.00 41.63	•	С
40	MOTA			23.568			1.00 41.91		С
	MOTA	2974 C		23.164			1.00 43.47		. 0
	ATOM	2975 0		24.784			1.00 46.52		N
	MOTA	2976 N					1.00 42.19		C
	MOTA		A ILE A 193	25.827			1.00 38.18		. c
45	MOTA		B ILE A 193	26.764			1.00 30.10		C
	ATOM	2982 C	G1 ILE A 193	26.159					C
	MOTA	2985 C	D1 ILE A 193	27.036			1.00 45.77		Ċ.
•	ATOM	2989	CG2 ILE A 193	27.961			1.00 42.22		
	ATOM	2993	: ILE A 193	26.603					C
50	MOTA	2994		27.213	-5.903	-8.984			0
20			N ARG A 194	26.596		-8.626			N .
	ATOM			27.234		3. -9.84 6	1.00 47.47		Ċ
	ATOM			26.904		-10.032			C
	MOTA		CB ARG A 194	27.273		-11.424			C C
	MOTA	•	CG ARG A 194			-11.320		٠.	Ċ
55	MOTA		CD ARG A 194	27.414	•	5 -12.548			N
• •	MOTA	_	NE ARG A 194	27.329					. C
	ATOM		CZ ARG A 194	27.59		7 -12.600			. O
. :	ATOM	3011	NH1 ARG A 194	27.96		-11.509		•	
	ATOM		NH2 ARG A 194	27.49		3 -13.742	1.00 51.03		N
60	ATOM		C ARG A 194	28.76					. C
UU	ATOM		O ARG A 194	29.33	1 -3.747	7 -10.924	1.00 57.83		0
	ATOM	2010	- 12.0 11 231						

_							00 400	2 241	0 703	1 00 40 22			N
5	ATOM .	3019	N	ARG A			29.433	-3.341	-8.723	1.00 49.23			
	ATOM.	3021	CA	ARG A			30.887	-3.378	-8.698	1.00 49.56			C
	ATOM	3023	CB	ARG A	195		31.470	-1.973	-8.965	1.00 49.15	•		С
	ATOM	3026	CG	ARG' A	195		32.684	-1.929	-9.832	1.00 45.49			Ç
	ATOM	3029	CD	ARG P			33.888	-1.211	-9.229	1.00 54.35			Ċ
10	ATOM	3032	NE	ARG A			33.658	0.142	-8.774	1.00 52.34			N
10	ATOM	3034	CZ	ARG F			34.625	0.982	-8.430	1.00 58.59	-		С
				ARG F			35.892	0.624	-8.476	1.00 59.01			N ·
	ATOM	3035		ARG I			34.335	2.210	-8.029	1.00 62.23			N
	MOTA	3038						-3.740	-7.314	1.00 51.05			C
	MOTA	3041		ARG A			31.317			1.00 31.03			ō
15	MOTA	3042	0	ARG A		•	30.795	-3.169	-6.362	1.00 52.25			N
	MOTA	3043	N	GLU A			32.281	•	-7.173				C
	MOTA	3045	CA	GLU A			32.723	-4.988	-5.831	1.00 53.43			C
	MOTA	3047	CB.	GLU A			33.192	-6.461	-5.735	1.00, 57.30			
•	MOTA	3050	CG	GLU A	196		32.048	-7.476	-5.923	1.00 59.93			C
20	MOTA	3053	CD	GLU A	196		32.485	-8.961	-5.919	1.00 65.83			С
	ATOM	3054	OE1	GLU A	196		32.977	-9.443	-6.966	1.00 59.79			0
	ATOM	3055		GLU A			32.327	-9.670	-4.885	1.00 64.02			0
	ATOM	3056	С		A 196		33.758	-3.977	-5.341	1.00 47.93			С
	ATOM	3057	ō	GLU A			34.933	-4.143	-5.563	1.00 45.07			0
25		3058	N		A 197	,	33.274	-2.911	-4.694	1.00 44.26			N
25	MOTA	3060	CA		A 197		34.115	-1.929	-4.021	1.00 39.52			С
	MOTA	3062		•	A 197		34.594	-0.730	-4.922	1.00 45.44			С
	ATOM						33.660	0.246	-5.517	1.00 40.87			C
	ATOM	3065	CG		A 197			0.002	-5.994				Č
	MOTA	3066		TRP A			32.438			1.00 45.72			N
30	ATOM.	3068		TRP A			31.860	1.157	-6.468	1.00 43.72			C
	MOTA	3070		TRP A			32.731	2.186	-6.302				C
	MOTA	3071		TRP 2			33.885	1.649	-5.705	1.00 45.88			<u></u>
	ATOM	3072	,	TRP			34.945	2.509	-5.427	1.00 46.01			Ċ
	MOTA	3074		TRP 2			34.813	3.842	-5.746	1.00 47.92			C
35	ATOM	3076	CH2	TRP	A 197		33.651	4.330	-6.338	1.00 50.66			С
	MOTA	3078	CZ2	TRP .	A 197		32.600	3.515	-6.626	1.00 43.28			С
	MOTA	3080	С	TRP .	A 197	•	33.334	-1.576	-2.764	1.00 38.50			С
•	ATOM	3081	0		A 197		33.528	-2.184	-1.733	1.00 49.55			.0
	ATOM	3082	·N	TYR .	A 198		32.472	-0.599	-2.786	1.00 38.10			N
40	ATOM	3084	CA		A 198		31.466	-0.531	-1.734	1.00 37.22			С
	ATOM	3086	СВ		A 198	•	30.770	0.851	-1.643	1.00 35.77			С
	ATOM	3089	. CG		A 198		31.675	2.028	-1.405	1.00 36.02			С
	ATOM	3090			A 198		31.813	2.562	-0.142	1.00 38.94			С
		3092			A 198		32.633	3.626	0.094	1.00 -39.66			С
45	ATOM	3094.	CZ		A 198		33.343	4.193	-0.948	1.00 44:31			С
43	ATOM	3094.	OH		A 198		34.174	5.269	-0.701	1.00 46.07	•		0
	ATOM	-					33.225	3.681	-2.233	1.00 44.86			C
	ATOM	3097			A 198			2.595	-2.448	1.00 42.57			Č
	ATOM	3099			A 198		32.386						c
	ATOM	3101	C		A 198		30.433		-2.214				.0
50	MOTA	3102	O.		A 198		30.574	-2.022	-3.287	1.00 30.84		•	
	ATOM	3103	N		A 199		29.405	-1.802	-1.418	1.00 38.45			N
	ATOM.	3105	CA	TYR	A 199		28.256	-2.557	-1.900	1.00 37.49	٠.		C
	ATOM	-3107	CB	TYR	A 199		27.490	-3.208	-0.728				С
	MOTA	3110	CG	TYR	A 199		28.233	-4.329	-0.047	1.00 32.48			С
55	MOTA	3111	CD1		A 199		28.787	-4.165	1.205	1.00 33.92			С
	ATOM	3113			A 199		29.453	-5.141	1.822	1.00 32.06			C.
	ATOM	3115	CZ		A 199		29.573		1.193	1.00 32.26			C
		3116	OH		A 199		30.243			1.00 34.61			0
	ATOM				A 199		29.024	-6.485	_				С
60	ATOM	3118			A 199		28.372			1.00 33.21			C
60	MOTA	3120					27.368						Ç
	ATOM	3122	C.	IIK	A 199	,	21.308	-1.323	2.043	1.00 30.31			Ÿ

WO 03/012089 PCT/GB02/03461

5	ATOM	3123	0	TYR A	199		26.418	-0.978	-2.075	1.00	45.22			. 0
•	ATOM	3124	N	GLU A			27.702	-1.272	-3.910	1.00	43.18		•	N
	ATOM	3126	CA	GLU A		•	27.054	-0.284	-4.777	1.00	43.16			С
	ATOM	3128	СВ	GLU A			28.089	0.193	-5.809		46.83			С
	ATOM	3131	CG	GLU A			27.626	1.383	-6.660	1.00	52.95			С
10 ·		3134	CD	GLU A	200		28.337	1.543	-7.977		51.92			С
	MOTA	3135	OE1	GLU A	200		29.496	1.164	-8.085		56.62			0
	ATOM	3136	OE2	GLU A	200		27.715	2.055	-8.901	1.00	54.72			0
	ATOM	3137	С	GLU A	200		25.857	-0.816	-5.577		44.00			С
	ATOM	3138	0	GLU A	200		25.993	-1.789	-6.319		48.61			Ο.
15	MOTA	3139	N	VAL A	201		24.691	-0.193	-5.481		37.72			N
	MOTA	3141	CA	VAL A	201		23.583	-0.713	-6.250		38.06		. 1	С
	ATOM	3143	CB	VAL A			22.598	-1.332	-5.374		33.81			C
	ATOM	3145		AYF Y			23.127	-2.629	-4.926		36.02			C
•	MOTA	3149		VAL A			22.411	-0.506	-4.261		33.46			C
20	MOTA	3153	С	VAL A			22.911	0.371	-7.006		36.84			C
	ATOM	3154	0	VAL A			23.235	1.474	-6.781		46.66			0
-	ATOM	3155	N	ILE A			21.975	0.073	-7.877		41.86			N
	ATOM	3157	CA	ILE A		•	21.271	1.122	-8.619		45.62			C
	MOTA	3159	CB	ILE A			21.435	0.898	-9.997		47.37			С
25	MOTA	3161		ILE A			22.924		-10.223		50.21			C
٠.	MOTA	3164		ILE A			23.240		-11.515		50.75			C
	ATOM	3168		ILE A			20.619		-10.700		47.14 46.10			C C
7	ATOM	3172		ILE A			19.779	1.335	-8.517				•	0
20	ATOM	3173	0.	ILE A			19.001	0.401	-8.788		46.34			N
30	ATOM	3174	N	ILE A			19.438	2.595	-8.195 -7.882		44.21			C
	ATOM	3176	CA	ILE A			18.092	3.089			42.75			c
	ATOM	3178	CB	ILE A			18.195	4.290	-6.931 -5.629		36.25	٠,		c
	ATOM	3180		ILE A			18.885	3.856 4.666	-3.629		37.62			c
35	ATOM	3183 3187		ILE A			16.754	4.972	-6.754		42.00			, C
33	MOTA MOTA	3191	CGZ	ILE A		•	17.508	3.646	-9.096		43.71			Ċ
	ATOM	3192	Ö	ILE A		-	18.164	4.384	-9.797		45.90			0
	MOTA	3193	N	VAL A			16.259	3.369	-9.374		43.96	•		N
	ATOM	3195		VAL A			15.807		-10.662		43.46			С
40	ATOM	3197	CB	VAL A			15.743		-11.563		47.55			С
	ATOM	3199		VAL A			17.031		-11.395		51.23			C
	ATOM	3203		VAL A			14.676		-11.133	1.00	52.39			Ċ
	MOTA	3207	·C	VAL A			14.525		-10.624		42.03			С
	ATOM	3208	0	VAL A			14.075	5.093	-11.639	1.00	46.48	•		. 0
45	ATOM	3209	N	ARG A	205		13.944	4.739	-9.445	1.00	40.50			N
	MOTEA	3211	CA.	ARG A	205		12.755	5.532	-9.254	1.00	41.19			С
	ATOM	3213	СВ	ARG A	205		11.567	4.685	-9.609	1.00	44.75			С
	MOTA	3216	CG	ARG A	205	•	10.235	5.385	-9.532	1.00	49.25			С
	MOTA	3219	CD	ARG A	205		9.191	4.670	-10.422	1.00	55.42		•	С
50	MOTA	3222	NE	ARG A	205		7.775	4.754	-10.007		57.55			N
	MOTA	3224	CZ	ARG A	205	:	6.805		-10.797	1.00	56.49			С
	ATOM	3225	NH1	ARG A	205		7.092		-12.017		54.80			N
	MOTA	3228	NH2	ARG A	205	•	5.550	5.215	-10.377		61.53	•		N
	MOTA	3231	С	ARG A			12.674	5.953	-7.799		38.57	•		С
55	MOTA	3232	Ο.	ARG A	205		13.264	5.307	-7.003	1.00	40.72			Ο.
	ATOM	3233	N	VAL A			11.961	7.032	-7.462		39.00			N
.*	-	3235	CA	VAL A			11.709	7.408	-6.072		35.25			C
	ATOM	3237	CB	VAL A			12.689	8.391			38.80			·C
	MOTA	3239		VAL A			12.331	8.891			40.25			. C
60	ATOM	3243		VAL A			14.073	7.800			45.84			C
	MOTA	3247	С	VAL A	206		10.285	8.022	-5.864	1.00	41.79			С

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5	ATOM	3356	CB	LYS A 214		9.120	13.673 -11.542		58.84			C
,	ATOM	3359	CG	LYS A 214		8.713	13.941 -12.984	1.00	63.68			C.
		3362	CD	LYS A 214		7.904	12.796 -13.625	1.00	65.33			C
	ATOM		CE	LYS A 214		8.338	12.533 -15.096	1.00	65.28			С
	MOTA	3365				7.187	12.419 -16.076		59.61			N
	MOTA	3368	NZ	LYS A 214		11.567	13.392 -11.355		54.17			С
10	ATOM	3372	С	LYS A 214			14.604 -11.251		59.68	•		0
	MOTA	3373	0	LYS A 214		11.617			56.61			N.
	MOTA	3374	N	MET A 215		12.632	12.628 -11.413		57.04			C
	MOTA	3376	CA	MET A 215		13.932	13.165 -11.741		57.19			c
	MOTA	3378	CB	MET A 215		14.810	13.356 -10.511					c
15	MOTA	3381	CG	MET A 215		14.273	14.458 -9.634		60.76			s
	ATOM	3384	SD	MET A 215		15.283	14.900 -8.238		63.39			C
	MOTA	3385	CE	MET A 215		16.644	15.670 -9.212		63.56			
	MOTA	3389	C	MET A 215		14.534	12.189 - 12.723		55.93			С
•	MOTA	3390	0	MET A 215		14.070	11.083 -12.896		51.96			0
20	ATOM	3391	N	ASP A 216		15.562	12.614 -13.410	1.00	58.57			N
20	ATOM	3393	CA	ASP A 216		16.199	11.718 -14.331		62.39			C.
		3395	СВ	ASP A 216		17.142	12.500 -15.225	1.00	64.34			С
	MOTA		CG	ASP A 216		18.371	11.744 -15.547	1.00	62.34			С
	MOTA	33.98		ASP A 216		18.562	10.659 -14.958		64.91			0
·	MOTA	3399		ASP A 216		19.194	12.167 -16.384		69.70			0
25	ATOM	3400				16.917	10.736 -13.424		63.11			С
	MOTA	3401	С	ASP A 216		17.563	11.142 -12.458		62:81			0
	ATOM	3402	0	ASP A 216			9.446 -13.708		64.18			N
	ATOM	3403	Ν.	CYS A 217		16.824			66.46		•	C.
	ATOM	3405	CA	CYS A 217		17.358	8.520 -12.735					Č
30	MOTA	3407	CB	CYS A 217		17.022	7.056 -13.051		66.11			š
	ATOM	3410	SG	CYS A 217		17.799	6.334 -14.479		72.28			C
	ATOM	3411	С	CYS A 217		18.822	8.755 -12.482		65.55			o
	ATOM	3412	0.	CYS A 217		19.283	8.527 -11.381		69.85			
	MOTA	3413	N	LYS A 218		19.547	9.255 -13.474		68.81			N
35	ATOM	3415	CA	LYS A 218		20.992	9.436 -13.327		70.13			C
,,,	ATOM	3417	CB	LYS A 218		21.618	10.160 -14.554	1.00	∵73.78	•		С
	ATOM	3420	CG	LYS A 218		22.335	9.229 -15.609	1.00	76.00			C
	MOTA	3423	CD	LYS A 218		23.033	9.987 -16.810	1.00	74.40			С
	ATOM	3426	CE	LYS A 218		23.953	9.050 -17.717	1.00	75.92			С
40	ATOM	3429	NZ	LYS A 218		23.299	7.995 -18.636		68.28			N
40	MOTA	3433	C	LYS A 218		21.288	10.204 -12.055		66.58			С
			ō	LYS A 218		22.340	10.059 -11.456		68.40			0
	ATOM	3434		GLU A 219		20.347	11.014 -11.621		61.73			N
	ATOM	3435.	N .	GLU A 219		20.604	11.871 -10.482		61.25			C.
45	MOTA	3437	CA	GLU A 219		19.634	13.041 -10.528	1.00	60.32			С
.45	ATOM	3439	CB				13.887 -11.782	1 00	65.08			С
-	ATOM	3442	CG	GLU A 219		19.746	14.781 -11.827		65.35			С
• *	ATOM -	3445	CD	GLU A 219		20.977			62.03			.0
	MOTA	3446		GLU A 219		21.905	14.598 -10.998			-		Ö
	MOTA	3447	OE2	2 GLU A 219		21.001	15.673 -12.717		0 68.30			Č
50	ATOM .	3448	C	GLU A 219		20.493			0 60.55			0
	ATOM	3449	0	GLU A 219		20.976	11.755 -8.113		0 60.04			
	ATOM ·	3450	N	TYR A 220		19.848	10.055 -9.051		0 58.43			N
	ATOM	3452	CA	TYR A 220		19.599	9.427 -7.771		0 54.98			С
	ATOM	3454	CB	TYR A 220		18.533	8.374 -7.903		0 56.27			C
55	ATOM	3457	CG	TYR A 220		17.175	8.915 -8.250	1.0	0.51.16			C
33	ATOM	3458	CD:			16.460		1.0	0 47.88			С
		3460			•	15.232			0 53.59			С
	ATOM		CZ	TYR A 220		14.696	•		0 54.76			С
	ATOM	3462		TYR A 220		13.443			0 59.59			0
C A	ATOM	3463		2 TYR A 220		15.390			0 45.89			С
60	MOTA	3465		2 MAD 1/ 33U		16.619			0 48.33			C
	MOTA	3467	CD	2 TYR A 220		10.019	J. J.J.J.					-

5	MOTA	3469	С	TYR	A 220		20.844	8.778	-7.324	1.00 55.05			С
	MOTA	3470	0	TYR	A 220		21.101	8.684	-6.135	1.00 58.11			
	MOTA	3471	N		A 221		21.616	8.340	-8.310	1.00 56.80			N
	ATOM	3473	CA	ASN	A 221		22.886	7.658	-8.110	1.00 56.10			C
	MOTA	3475	·CB	ASN	A 221		22.874	6.380	-8.928	1.00 51.38			č
10	ATOM	3478	CG		A 221		21.838	5.430	-8.435				c
	ATOM	3479			A 221		, 21.923	4.970	-7.294	1.00 54.95			0
	ATOM	3480			A 221		20.830	5.136	-9.272	1.00 50.76			
	ATOM	3483	C		A 221		24.068	8.511					N
•	ATOM	3484	ŏ		A 221				-8.521	1.00 59.72			C
15	ATOM	3485	N		A 222		25.123 23.909	7.989		1.00 63.63			0
15	ATOM	3487	CA		A 222			9.823	-8.393	1.00 63.40			N
	ATOM	3489					24.919	10.707	-8.917	1.00 63.06			C.
			CB		A 222		24.506	12.178	-9.007	1.00 68.66			С
	ATOM	3492	CG		A 222		25,696	13.048	-9.334	1.00 67.88			С
20	ATOM	. 3493			A 222		26.577		-10.333	1.00 72.26			С
20	ATOM	3495			A 222		27.666		-10.632	1.00 77.81			С
	ATOM	3497	CZ		A 222		27.889	14.606	-9.925	1.00 79.75			С
	ATOM	3498	OH		A 222		28.992	15.374	-10.239	1.00 83.62			0
	ATOM	3500			A 222		27.018	14.993	-8.917	1.00 75.27			c ·
	ATOM	3502	CD2	TYR .	A 222		25.942	14.216	-8.632	1.00 69.85			С
25	MOTA	3504	С	TYR .	A 222		26.139	10.534	-8.091	1.00 61.93		٠,	c
	MOTA	3505	0	TYR .	A 222		26.223	10.993	-6.934	1.00 51.08			ō
	ATOM	3506	N	ASP .	A 223		27.055	9.829	-8.771	1.00 65.98			N
	ATOM	3508	CA		A 223		28.389	9.416	-8.349	1.00 58.22			C
	ATOM	3510	CB		A 223			10.429	-7.382	1.00 58.25	•		c
30	ATOM	3513	CG		A 223	•	29.709		-6.239	1.00 50.25			c
	ATOM	3514			A 223		28.983	9.249	-5.377	1.00 75.60			o
	ATOM	3515			A 223		30.956	9.791	-6.110	1.00 75.00			
	ATOM	3516	C .		A 223		28.238	7.959	-7.885	1.00 56.27			0
	ATOM	3517	ō		A 223		28.790	7.052	-8.514				C
35	ATOM	3518	N		A 224		27.463	7.710		1.00 48.60			0
	ATOM	3520	CA		A 224		27.203	6.317	-6.829	1.00 60.43			N
	ATOM	3522	CB		A 224		28.440		-6.389	1.00 58.39			C
	ATOM	3525	CG		A 224		28.722	5.692	-5.784	1.00 55.03			C
	ATOM	3528	CD		A 224			6.175	-4.403	1.00 53.98			С
40	ATOM	3531	CE		A 224		30.039	5.591	-3.910	1.00 51.13			С
,	MOTA	3534	NZ				30.576	6.430	-2.777	1.00 50.78			С
	ATOM	3538			A 224		30.830	7.806	-3.279	1.00 52.27			N
		3539	С		A 224		26.093	6.132	-5.382	1.00 57.12			С
	MOTA	3540	0		A 224		25.621	7.085	-4.735	1.00 59.55			0
45	MOTA		N		A 225		25.697	4.870	-5.246	1.00 56.45			N
· 1 3	MOTA	3542	CA		A 225		24.636	4.461	-4.316	1.00 52.86			С
	MOTA	3544	CB		A 225		23.338		-5.076	1.00 50.03		. (С
	MOTA	3547	OG		A 225		22.661	5.516		1.00 52.69		(0
	MOTA	3549	С		A 225		25.040	3.197	-3.570	1.00 48.24		. (С
50	MOTA	3550	0	SER A			25.422	2.202	-4.180	1.00 48.80		. (Э
.50	MOTA	3551	N		A 226		24.969	3.241	-2.244	1.00 44.93		7	N
	ATOM	3553	CA		A 226		25.441	2.125	-1.454	1.00 37.58			С
	MOTA	3555	CB	ILE A	A 226			2.379	-1.017	1.00 39.22			С
•	ATOM	3557	CG1	ILE A	A 226		26.923	3.507	-0.005	1.00 37.98			C
	MOTA	3560	CD1	ILE A	A 226		28.301	3.756	0.555	1.00 34.23			Ċ.
55	MOTA	3564		ILE A		•	27.756	2.690	-2.212	1.00 38.02			C
	MOTA	3568	С		A 226		24.632	1.817	-0.239	1.00 38.95			C
	ATOM	3569	0	ILE A			23.774	2.567	0.185	1.00 38.93	•		o
	ATOM	3570	N	VAL A			24.920	0.635	0.310	1.00 47.23			
	ATOM	3572		VAL A			24.282	0.137	1.528	1.00 40.07			N
60	ATOM	3574	CB	VAL A			23.835	-1.340	1.328	1.00 39.95			C
	ATOM	3576		VAL A			23.223	-1.863	2.677		•		C
				2				1.003	2.011	1.00 42.20		(С

		7									
5	. ATOM	3580	CG2	VAL 2	A 227		22.852	-1.446	0.279	1.00 32.66	С
•	ATOM	3584	С	VAL 2	A 227		25.298	0.175	2.644		
	MOTA	3585	0	VAL	A 227		26.400	-0.407	2.485	1.00 31.57	0
	MOTA	3586	N	ASP 2	A 228		24.951	0.813	3.768	1.00 42.83	N
	ATOM	3588	CA	ASP 2	A 228		25.934	0.901	4.892	1.00 44.00	С
10	ATOM	3590	CB	ASP 2	A 228		26.926	2.001	4.665	1.00 47.22	С
	ATOM	3593	CG	ASP 2	A 228		27.484	2.542	5.943	1.00 55.34	· C
•	ATOM	3594	OD1	ASP 2	A 228		27.322	1.886	6.990	1.00 60.37	. 0
	ATOM	3595	OD2	ASP 3	A 228		28.093	3.631	6:003	1.00 65.03	0
	ATOM	3596	С	ASP 2	A 228		25.364	1.037	6.287	1.00 43.99	С
15	ATOM	.3597	0	ASP :	A 228		24.829	2.037	6.705	1.00 43.43	Ο.
	ATOM	3598	N	SER 2	A 229		25.535	-0.057	6.977	1.00 45.99	N
	MOTA	3600	CA	SER .	A 229		25.113	-0.268	8.307	1.00 43.77	С
	MOTA	3602	CB	SER .	A 229		25.400	-1.715	8.589	1.00 43.80	C
•	ATOM	3605	OG	SER .	A 229		26.786	-1.836	8.462	1.00 43.49	. О
20	ATOM	3607.	С	SER .	A 229		25.987	0.478	9.228	1.00 39.36	С
	ATOM	3608	0	SER .	A 229		25.806	0.377	10.394	1.00 35.35	0
	ATOM	3609	N	GLY .	A 230		26.982	1.181	8.705	1.00 40.62	. N
	ATOM	3611	CA	GLY .	A 230		27.805	2.105	9.509	1.00 37.16	. C
	ATOM	3614	C		A 230		27.388	3.543	9.319	1.00 38.50	. С
25	MOTA	3615	o		A 230		28.040	4.500	9.740	1.00 38.84	. 0
	ATOM	·3616	N	THR	A 231		26.265	3.690	8.657	1.00 36.83	N
	ATOM	3618	CA	THR	A 231		25.672	4.981	8.477	1.00 36.29	С
	ATOM	3620	СВ		A 231		25.795	5.339	7.037	1.00 36.20	С
	ATOM	3622	OG1	THR	A 231		27.141	5.728	6.829	1.00 32.63	. 0
30	ATOM	3624	CG2	THR	A 231		24.980	6.570	6.709	1.00 33.65	Ç
	MOTA	3628	С	THR .	A 231		24.231	4.977	8.968	1.00 36.96	. С
	MOTA	3629	0	THR	A 231		23.479	4.036	8.702	1.00 36.51	0
	ATOM	3630	N	THR	A 232		23.868	6.048	9.672	1.00 39.63	N
	ATOM	3632	CA	THR	A 232		22.586	6.197	10.378	1.00 44.48	С
35	ATOM	3634	CB	THR	A 232		22.776	7.362	11.370	1.00.47.87	С
	ATOM	3636	OG1	THR	A 232		23.819	7.053	12.305	1.00 58.32	0
	ATOM	3638	CG2	THR	A 232		21.553	7.610	12.240	1.00 52.16	. С
	MOTA	3642	С	THR	A 232		21.384	6.554	9.507	1.00 46.65	С
	ATOM	3643	0	THR	A 232		20.315	5.954	9.593	1.00 48.65	0
40	MOTA	3644	N	ASN	A 233		21.590	7.547	8.663	1.00 47.89	N-
	ATOM	3646	CA	ASN	A 233		20.523	8.231	7.983	1.00 47.43	С
	MOTA	3648	СВ		A 233		20.878	9.715	7.971	1.00 48.12	С
	MOTA	3651	CG	ASN	A 233		20.435	10.435	9.198	1.00 43.02	С
	MOTA	3652			A 233		20.365	9.883	10.276	1.00 38.96	0
45	MOTA .	3653	ND2		A 233		20.145	11.703	9.035	1.00 50.70	Ŋ
	ATOM	3656	С		A 233		20.451	7.803	6.572	1.00 48.67	c
	MOTA	3657	0		A 233		21.360	7.093	6.131	1.00 51.81	0
	MOTA	3658	N		A .234		19.403	8.234	5.856		N
	MOTA	3660	CA		A 234		19.333	7.999		1.00 46.15	C
50·	MOTA	3662	CB	LEU	A 234	•	17.912		3.895	1.00 46.39	. C
	MOTA	3665	CG		A 234		17.655	7.385	2.424		С
٠.	MOTA	3667			A 234		16.562	8.293			
	MOTA	3671	CD2	LEU	A 234		18.868	7.415	1.522	1.00 47.77	C
	ATOM	367.5	C		A 234		19.842	9.286	3.867	1.00 45.80	C
55	ATOM -	3676	0		A 234		19.245	10.301	4.146	1.00 51.40	0
	ATOM	3677	N ·	ARG	A 235		20.940	9.231	3.104	1.00 47.98	N
-	MOTA	3679	CA		A 235		21.555	10.393	2.452	1.00 41.53	. С
	ATOM	3681	CB		A 235		23.058	10.339	2.514	1.00 40.87	. С
	ATOM	3684	CG.		A 235		23.653	9.849		1.00 41.40	C
60	MOTA	3687	· CD		A 235		23.645	10.825	4.775	1.00 46.10	, C
	ATOM	3690	NE.	ARG	A 235		24.981	11.103	5.305	1.00 52.10	N

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5	ATOM	3692	CZ	ARG A 235		25.469	12.342	5.380		54.49			(
-	ATOM	3693		ARG A 235		26.649	12.577	5.870		51.49				N
	ATOM	3696		ARG A 235		24.751	13.366	4.949	1.00	62.47				N
	ATOM	3699		ARG A 235		21.284	10.362	0.984		42.47				C
	ATOM	3700		ARG A 235		21.322	9.234	0.354		35.71				0
10		3701		LEU A 236		21.054	11.575	0.446	1.00	42.38				N
10	_ATOM	3703		LEU A 236		20.755	11,710	-0.959	1.00	44.15				C
	ATOM			LEU A 236		19.287	12.033	-1.112	1.00	46.30			(С
	ATOM	3705		LEU A 236		18.420	11.070	-0.325		46.08			(С
	ATOM	3708		LEU A 236		17.143	11.742	0.192		50.37				С
	MOTA	3710		LEU A 236		18.143	9.851	-1.201		46.39				Ċ Ċ
15	ATOM	3714				21.574	12.774	-1.606		46.18				С
	ATOM	3718		LEU A 236			13.760	-1.003		56.50				o`
	ATOM	3719		LEU A 236		21.974 21.861	12.556	-2.850		43.50				N
	MOTA	3720		PRO A 237			13.586	-3.669		48.09				С
- i	MOTA	3721	CA	PRO A 237		22.474	13.003	-5.075		50.44				c
20	MOTA	3723	CB	PRO A 237		22.378	11.517	-4.873		47.91				Ç.
	MOTA	3726	CG	PRO A 237		22.263	11.287	-3.541		43.62				Ċ
	ATOM .	3729	ĊD	PRO A 237		21.677	14.854	-3.533		47.59				C
	MOTA	3732	С	PRO A 237		21.657		-3.621		56.42				ō
	ATOM	3733	0	PRO A 237		20.443	14.793	-3.340		54.44				N
25 ·	MOTA	3734	N	LYS A 238		22.324	15.977	-2.966		59.43				C
	MOTA	3736	CA	LYS A 238		21.710	17.262	-3.006		65.19				c
	ATOM	3738	CB	LYS A 238		22.759	18.345	-2.056		68.51		.*		c
	MOTA	3741	CG	LYS A 238		22.458	19.459			69.31				c
	ATOM	3744	CD	LYS A 238		21.616	20.524	-2.702		74.63				c
30	ATOM	3747	CE.	LYS A 238		21.206	21.491	-1.626		72.38				Ň
	MOTA	3750	NZ	LYS A 238		21.148	20.760	-0.296		60.04				C
	ATOM	3754	С	LYS A 238		20.530	17.740	-3.770		62.70				ŏ
	MOTA	3755	0	LYS A 238		19.535	18.188	-3.218		61.99				N
	MOTA	3756	N	LYS A 239		20.645	17.681	-5.078		62.06			-	C
35	ATOM	3758	CA	LYS A 239		19.502	17.942	-5.889		65.93			•	c
	MOTA	3760	ĆB	LYS A 239		19.803	17.627	-7.373		69.24				Ç.
	ATOM	3763	CG	LYS A 239		19.794	18:830	-8.411		71.82				c
	ATOM.	3766	CD	LYS A 239		21.071	18.808	-9.350						C
	ATOM	3769	CE	LYS A 239		20.782		-10.877		73.55				N
40	MOTA	3772	NZ	LYS A 239		21.914		-11.760		70.78				C
	MOTA	3776	C	LYS A 239		18.444	16.999	-5.285		64.24				ŏ
	ATOM	3777	0	LYS A 239		17.406	17.455	-4.781		68.73				N
	MOTA	3778	N	VAL A 240		18.705	15.691	-5.278		58.91				C
	MOTA	3780	CA	VAL A 240		17.635	14.751	-4.914		62.19				C.
45	MOTA	3782	CB	VAL A 240		18.084	13.284	-4.909		65.97				c
	MOTA	3784		VAL A 240		16.867		-4.847		66.12				c
	MOTA	3788	CG2	VAL A 240		18.913	12.947	-6.147	_	68.39				c
	MOTA	3792	Ċ	VAL A 240		17.034	15.079	-3.556		58.68				
	MOTA	3793	. 0	VAL A 240		15.811		-3.379		54.40				0
50	.ATOM	3794	N	PHE A 241		17.906		-2.587		56.41				N
	ATOM	3796	CA	PHE A 241			15.677	-1.278		52.63				C
	MOTA	3798	CB	PHE A 241		18.635		-0.376		50.48	•			C
	ATOM	3801	CG	PHE A 241		18.276		0.957		50.54	•			·C
	ATOM	. 3802	CD1	PHE A 241		17.615	15.854	1.945		53.71		•		C
55	ATOM	3804	CE1	PHE A 241		17.303		3.181		54.61				C
	ATOM -	3806	CZ	PHE A 241	•	17.662		3.427		55.24				C
	ATOM	3808	CE2	PHE A 241		18.322		2.440		55.17				C
	ATOM	3810	CD2	PHE A 241		18.624				0 57.01				C
	ATOM	3812		PHE A 241		16.561				0 51.84	•			C
60	ATOM	3813		PHE A 241		15.439				0 47.71				0
	ATOM	3814		GLU A 242		17.031	17.857	-2.245	1.0	0 53.89				N

5	ATOM	3816	CA		A 242		19.085	-2.353	1.00 56.53	. · c
	ATOM	3818	CB		A 242		20.110	-3.362	1.00 59.79	
	MOTA	3821	CG		A 242		21.353	-2.697	1.00 66.19	С
	MOTA	3824	CD	GLU	A 242	2 17.130	21.454	-1.185	1.00 74.63	С
	ATOM	3825			A 242			-0.789	1.00 79.35	0
10	ATOM	3826	OE2	GLU	A 242	18.091	21.487	-0.372	1.00 76.40	0
	MOTA	3827	С	GLU	A 242	2 14.790	18.768	-2.638	1.00 53.63	С
	ATOM	3828	Ó	GLU	A 242	2 13.937	19.203	-1.880	1.00 45.24	0
•	ATOM	3829	N		A 243		17.997	-3.709	1.00 52.72	N
· . · .	ATOM	3831	CA		A 243		17.599	-4.140	1.00 50.49	C
15	MOTA	3833	CB	ALA	A 243	13.258	16.838	∸5.428	1.00 51.48	С
	MOTA	3837	C.	ALA	A 243	12.383	16.781	-3.120	1.00 51.02	С
	MOTA	3838	O	ALA	A 243	11.259	17.157	-2.763	1.00 54.64	. 0
	ATOM	3839	N	ALA	A 244	12,949	15.670	-2.653	1.00 46.51	N
	MOTA	3841	CA	ALA	A 244	12.262	14.833	-1.670	1.00 41.75	. С
20	MOTA	3843	CB		A 244		13.694	-1.156	1.00 37.69	, , C
	MOTA	3847	С	ALA	A 244	11.792	15.630	-0.490	1.00 44.76	C
•	MOTA	3848	0	ALA	A 244	10.658	15.496	-0.084	1.00 47.71	0
	MOTA	3849	N	VAL	A 245	12.646	16.470	0.083	1.00 52.14	N
• .	MOTA	3851	CA	VAL	A 245	12.279		1.348	1.00 53.69	C
25	MOTA	3853	CB	VAL	A 245			1.854	1.00 53.93	C
	MOTA	3855	CG1	VAL	A 245	12.824	18.785	3.121	1.00 53.73	C
	MOTA	3859	CG2	VAL	A 245			2.106	1.00 58.55	. c
	ATOM	3863	С	VAL	A 245	10.976		1.141	1.00 52.68	Ċ
	MOTA	3864	0	VAL	A 245	10.072		1.976	1.00 57.49	ō
30	ATOM	3865	N	LYS	A 246	10.904	18.444	-0.015	1.00 49.32	N
	ATOM	3867	CA	LYS	A 246	9.816		-0.367	1.00 54.20	Ċ
	ATOM	3869	CB	LYS	A 246	10.200	19.988	-1.684	1.00 58.55	. C
	ATOM .	3872	CG	LYS	A 246			-1:943	1.00 63.23	
·	MOTA	3875	CD	LYS	A 246	12.640	21.041	-1.337	1.00 70.71	C
35	ATOM	3878	CE	LYS	A 246	13.228	20.765	0.055	1.00 70.11	· C
	ATOM	3881	NZ	LYS	A 246	13.337		0.860	1.00 70.79	. N
	- ATOM	3885	С	LYS	A 246	8.550	18.497	-0.458	1.00 56.50	C
	MOTA	3886	0	LYS	A 246	7.635		0.345	1.00 62.61	0
	MOTA	3887	N	SER	A 247	8.510	17.574	-1.417	1.00 53.80	N
40	ATOM	3889	CA	SER	A 247	7.381	16.674	-1.534	1.00 45.07	С
•	MOTA	3891	CB	SER	A 247	7.699	15.537	-2.496	1.00 45.02	С
	ATOM	3894	OG	SER	A 247		14.587	-2.462	1.00 43.14	0
•	ATOM	3896	С	SER .	A 247	7.010	16.123	-0.162	1.00 38.07	С
	MOTA	3897	0	SER	A 247	5.842	15.925	0.137	1.00 47.02	0
45 ·	MOTA	3898	N	ILE .	A 248	8.008	15.906	0.685	1.00 35.51	Ń
	MOTA	3900	CA	ILE .	A 248	7.738	15.379	2.012	1.00 44.04	С
	MOTA	3902	CB		A 248		14.787	2.672	1.00 45.65	С
	MOTA	3904			A 248		13.394	2.080	1.00 38.16	С
	MOTA	3907			A 248	10.760		2.337	1.00 33.98	.C
50	ATOM	3911	CG2	ILE !	A 248	8.970	. 14.588	4.187	1.00 46.92	. C
	MOTA	3915	С	ILE .	A 248		16.401	2.846	1.00 51.15	· c
	MOTA	3916	0	ILE .	A 248	6.052	16.024	3.606	1.00 56.50	0
	MOTA	3917	N.	LYS .	A 249	7.281	17.689	2.671	1.00 53.92	N
•	MOTA	3919	CA	LYS	A 249	6.627		3.389	1.00 54.59	C.
55	MOTA	3921	CB	LYS :	A 249		20.147		1.00 58.74	Ċ
	ATOM	3924			A 249		20.554	3.850	1.00 58.89	· č
	ATOM	3927			A 249		21.880	3.249	1.00 58.57	· c
	MOTA	3930			A 249		22.330	3.774	1.00 61.39	č
	MOTA	3933			A 249		22.849	2.647	1.00 57.83	N
60	MOTA	3937			A 249		18.935	2.964	1.00 54.92	c
	MOTA	3938			A 249		18.932	3.790	1.00 54.00	Ö
•		•								U

5	ATOM	3939	N	ALA A 250		5.003	19.083	1.656	1.00 49.70			N
	MOTA	3941	_	ALA A 250		3.688	19.218	1.060	1.00 52.00			C
	MOTA	3943		ALA A 250		3.786		-0.465	1.00 53.40			C
	ATOM	3947		ALA A 250		2.773	18.163	1.636	1.00 53.09			C
	MOTA	3948		ALA A 250		1.602	18.407	1.922	1.00 60.66			0
10	ATOM	3949	•	ALA A 251	•	3.344	16.980	1.805	1.00 57.05			N
	ATOM	3951		ALA A 251		2.639	15.818	2.338	1.00 55.70			C
	MOTA	3953		ALA A 251		3.420	14.558	1.986	1.00 53.52			
	MOTA	3957		ALA A 251	•	2.404	15.877	3.856	1.00 58.05			C 0
	ATOM	3958		ALA A. 251		1,461	15.323	4.372	1.00 62.89	• *		. И.
15	MOTA	3959	_	SER A 252		3.281	16.529	4.590	1.00 59.77			C
	ATOM.	3961	CA	SER A 252		3.147	16.572	6.034	1.00 56.96			C
	MOTA	3963	CB	SER A 252		4.562	16.585	6.606	1.00 59.16			o
	ATOM	3966		SER A 252		5.524	16.922	5.592	1.00 58.00			C
•	MOTA	3968	C	SER A 252		2.413	17.837	, 6.419	1.00 56.47			0
20	ATOM	3969	0	SER A 252		2.110	18.098	7.575	1.00 51.08	,		N
-	ATOM	3970	N	SER A 253		2.089	18.610	5.401	1.00 59.91		٠.	C
	MOTA	3972	CA	SER A 253		1.690	20.003	5.568	1.00 59.18			C
	ATOM	3974	CB	SER A-253		1.581	20.643	4.173	1.00 57.63			Ö
	ATOM	. 3977	OG	SER A 253		1.316	22.026	4.257	1.00 55.74			c
25	MOTA	3979	С	SER A 253		0.484	20.373	6.441	1.00 60.11			ŏ
	MOTA	3980	Ο.	SER A 253		0.075	21.526	6.428	1.00 59.14 1.00 60.35			И
	MOTA	3981	N	THR A 254		-0.099	19.451	7.200				C
	MOTA	3983	CA	THR A 254		-1.147	19.897		1.00 60.80 1.00 60.71			Č
	MOTA	3985	CB	THR A 254		-2.318	18.951	8.293	1.00 56.78			0
30	MOTA	3987 ·		THR A 254		-1.905	17.797	9.043	1.00 56.78			C
	ATOM	3989		THR A 254		-2.858	18.465	6.955	1.00 64.58			C.
	ATOM	3993	C	THR A 254		-0.473	20.059	9.435	1.00 68.02		•	0
	MOTA	3994	0	THR A 254		-1.121	20.164	10.478 9.385	1.00 66.30			N
خد	MOTA	3995	N	GLU A 255		0.848	20.400	10.537	•			C
35	ATOM	3997	CA	GLU A 255		1.626 1.998	19.192	11.398	1.00 70.30			· C
	MOTA	3999	CB	GLU A 255		0.804	18.717	12.245	1.00.70.88			С
	MOTA	4002	CG	GLU A 255 GLU A 255		1.164	18.170	13.624	1.00 72.29			С
	ATOM	4005	CD	GLU A 255		2.307	18.397	14.115	1.00 79.50			0
40	ATOM	4006		GLU A 255		0.285	17.519	14.229	1.00 62.93	•		0
40	MOTA	4007 4008	C	GLU A 255		2.810	21.164	10.000	1.00 72.57			С
	MOTA	4008	Ö	GLU A 255		3.248	20.966	8.852	1.00 74.27			0
	MOTA	4010	N	LYS A 256		3.298	22.083	10.818	1.00 72.10			N
	MOTA	4012	CA	LYS A 256		4.408	22.901	10.411	1.00 68.65			С
45	ATOM ATOM	4012	CB	LYS A 256		4.017	24.356	10.254	1.00 69.61			С
73	ATOM	4017	CG	LYS A 256		3.138	24.580	9.037	1.00 76.54			С
	ATOM	4020	CD	LYS A 256		3.813	24.086	7.737	1.00 79.94			С
	ATOM	4023	CE	LYS A 256		3.261	24.791	6.471	1.00 79.27			С
	ATOM	4026	NZ	LYS A 256		2.321	23.945	5.676	1.00 79.72			N
50	ATOM	4030	C	LYS A 256		5.429		11.462	1.00 64.96			С
.50	ATOM	4031	ŏ	LYS A 256		5.097		12.658	1.00 51.53			. 0
	ATOM	4032	N	PHE A 257		6.664		10.972	1.00 61.73		•	N
	ATOM	4034	CA	PHE A 257		7.826		11.762	1.00 60.99			С
	ATOM	4036	СВ	PHE A 257		8.370	_	11.354	1.00 65.88			С
55	ATOM	4039	CG	PHE A 257		7.338		11.397	1.00 67.36		•	·C
	ATOM	4040		PHE A 257		6.875		10.232	1.00 71.73			С
	ATOM	4042		PHE A 257		5.931		10.278	1.00 72.34			С
	MOTA	4044	CZ	PHE A 257		5.447		11.503				С
	MOTA	4046		PHE A 257		5.910	18.476 [.]	12.667				С
60	ATOM	4048	_	PHE A 257		6.840	19.469	12.611				С
	ATOM	4050		PHE A 257		8.811	23.466	11.392	1.00 59.35			С

_	7.0014	4051	· ·	PHE A	257		8.716	24.049	10.333	1.00	58.22			0	
5	ATOM	4051		PRO A			9.766				61.91			N	
	MOTA	4052	-				10.792	24.731	11.983		65.38			С	
•	MOTA	4053		PRO A					13.358		66.17			C	
	MOTA	4055		PRO A			11.351	25.053			64.85			c	
	MOTA	4058		PRO A			10.803	23.979	14.309		61.29			č	
10	MOTA	4061		PRO A			9.949	23.054	13.546					c	
	MOTA	4064	С	PRO A	258		11.875	24.094	11.144	1.00	69.63				
	MOTA	4065	0 -	PRO A	258		12.156	22.912	11.335		67.19			0	
	ATOM	4066	N	ASP A	259		12.485	24.858	10.248		74.52	•		N	
	ATOM	4068	CA	ASP A	259		13.450	24.293	9.308	1.00	76.21			С	•
15	MOTA	4070	СВ	ASP A	259		14.038	25.411	8.459	1.00	78.78			С	•
••	ATOM	4073		ASP A			12.952	26.362	7.934	1.00	85.56			. C	
	ATOM	4074		ASP A			12.355	26.110	6.853		85.56			0	
	ATOM	4075		ASP A			12.604	27.384	8.566		94.62			О	
•	ATOM	4076		ASP A			14.514	23.433	10.009	1.00	75.34			С	
20	MOTA	4077		ASP A			14.811	22.315	9.560	1.00	77.54			Ο,	
20		4078		GLY A			15.056	23.927	11.119	1.00	68.42			N	
	MOTA	4070		GLY A			16.038	23.173	11.867	1.00	65.64			С	
	ATOM			GLY A		•	15.782	21.681	11.757		64.85			С	
	MOTA	4083		GLY A			16.705	20.864	11.545		65.50			0	
0.5	MOTA	4084					14.512	21.331	11.912		62.03			N	
25	MOTA	4085	N	PHE A			14.039	19.953	11.778		60.14			С	
	MOTA	4087	CA	PHE A			12.545	19.893	12.146		59.84			С	
	MOTA	4089	CB	PHE A			11.901	18.542	11.976		53.88			С	
	MOTA	4092	CG	PHE A			12.040	17.584	12.931		50.78			Ċ	
	MOTA	4093		PHE A			11.450	16.369	12.790		51.53			C	
30	ATOM	4095		PHE A			10.699	16.096	11.676		55.50			С	
	MOTA	4097	CZ	PHE A			10.542	17.043	10.705		51.48			С	
	ATOM	4099		PHE A			11.140	18.260	10.859		55.00			. c	
	ATOM	4101		PHE A			14.271	19.432	10.364		60.30			С	
25	ATOM	4103	С	PHE A			14.921	18.396	10.165		62.84			. 0	
35	ATOM	4104	O N	TRP A		•	13.778	20.132	9.363		52.97			N	
	MOTA	4105	N	TRP A			13.930	19.551	8.071		54.85			C	
	MOTA	4107	CA CB	TRP A			13.154	20.339	7.017		56.23			С	
	MOTA	4109	CG	TRP A		•	11,652	20.135	7.269		61.23			С	
40	MOTA	4112		TRP A			10.780	21.050	7.761		66.49			С	
40 .	ATOM	4113 4115		TRP A			9.525	20.510	7.874		68.50			N	
	MOTA	4117		TRP A			9.565	19.213	7.447		67.88			. C	
	ATOM			TRP A			10.889	18.941	7.064		61.30			C	
	ATOM	4118		TRP A			11.188	17.669	6.586		64.17			С	
15	ATOM	4119		TRP F			10.177	16.728	6.510		63.85			С	:
45	ATOM	4121		TRP F			8.879	17.034	6.896		66.57	•		С	:
	MOTA	4123		TRP F			8.547	18.266			66.36		•	С	
	ATOM	4125	C	TRP F			15.391	19.391	7.785		53.56			C	
	MOTA	4127	-				15.769		6.757		56.81			.0)
50	MOTA	4128	0	TRP A	202		16.220		8.725		58.44			N	I
50	ATOM	4129	N.	LEU A			17.677		8.531		58.98			. c	
	MOTA	4131	CA	LEU A			18.170				57.08			Ċ	
:	MOTA	4133	CB	LEU A			18.031		7.709		59.71			Ċ	
٠٠.	MOTA	4136		LEU A					8.206		59.96			Ċ	
	MOTA	4138		LEU A			18.483				0 60.81	•		Ċ	:
55	MOTA	4142		LEU 1			18.875				0 62.54			. ,	:
	MOTA	4146	С.		A 263		18.468		_		0 61.58			ò	
	MOTA	4147	0		A 263		19.686				0 67.37			. 1	
	MOTA	4148	N		A 264		17.778							ç	
	MOTA	4150			A 264		18.436				0 70.18 0 72.26				Š
60	MOTA	4153			A 264		18.788))
	MOTA	4154	0	GLY A	A 264		18.910	17.143	13.194	1.0	0 76.04			`	٠.

								10 140	1 00 71 03				N
5	ATOM.	4155	N	GLU A 265		18.927	19.149	12.149	1.00 71.01				C
	MOTA	4157	CA.	GLU A 265		19.437		13.311	1.00 71.40				
	ATOM	4159	СВ	GLU A 265		19.648	21.383		1.00 71.95				C.
	ATOM	4162	CG	GLU A 265		20.982	21.698	12.353	1.00 74.37				C
	MOTA	4165	CD	GLU A 265		20.958	22.955	11.471	1.00 74.89				C
10	ATOM	4166		GLU A 265		21.757	23.022	10.500	1.00 63.91				0
10	ATOM	4167		GLU A 265		20.142	23.876	11.745	1.00 80.45				0
	ATOM	4168	C	GLU A 265		18.592	19.716	14.547	1.00 70.60				С
		4169	ō	GLU A 265		19.099	19.216	15.542	1:00 72.28				0
	ATOM	4170	N	GLN A 266		17.322	20.118	14.516	1.00 68.36				N
10	ATOM			GLN A 266		16.574	20.094	15.769	1.00 68.13				С
15	MOTA	4172	CA	GLN A 266		16.036	21.431	16.254	1.00 71.81				C
	MOTA	4174	CB	GLN A 266		15.288	22.275	15.282	1.00 73.46				С
	MOTA	4177 .	CG			15.211	23.702	15.831	1.00 80.14				С
	MOTA	4180		GLN A 266			24.530	15.578	1.00 78.16				0
	MOTA	4181		GLN A 266		16.098		16.604	1.00 81.99				N
20	MOTA .	4182		GLN A 266		14.163	23.982	15.770	1.00 65.19				С
	MOTA	4185	С	GLN A 266		15.495	19.132		1.00 68.32				ō
	MOTA	4186	0	GLN A 266		14.952	18.739	14.761	1.00 62.13				N
	ATOM	4187	N	LEU A 267		15.179	18.751	16.973					C
	ATOM	4189	CA	LEU A 267		14.400	17.604	17.135	1.00 60.81				c
25	ATOM	4191	CB	LEU A 267		14.990	16.849	18.335	1.00 60.23				c
	MOTA	4194	CG	LEU A 267		14.662	17.271	19.724	1.00 56.50				
	ATOM	4196	CD1	LEU A 267		13.130	17.340	19.756	1.00 54.80				C
	MOTA	4200	CD2	LEU A 267		15.234	16.210	20.656	1.00 52.66				C
	ATOM	4204		LEU A 267		12.988	18.098	17.205	1.00 60.54				C
30	ATOM	4205	0			12.771	19.279	17.110	1.00 67.47				0
30	ATOM	4206	N	VAL A 268		12.013	17.214	17.315	1.00 67.35				N
	ATOM	4208	CA	VAL A 268		10.617	17.635	17.398	1.00 64.13				С
	MOTA	4210	СВ	VAL A 268		9.915	17.517	16.071	1.00 64.12				С
	ATOM	4212		VAL A 268	٠,	8.431	17.553	16.280	1.00.64.85				C.
35	ATOM	4216	CG2	VAL A 268		. 10.332	18.629	15.148	1.00 68.52				C
55	MOTA	4220	C	VAL A 268		9.895	16.719	18.348	1.00 65.02			٠	С
	MOTA	4221	.0	VAL A 268		10.339	15.595	18.595	1.00 67.72				0
		4222	N	CYS A 269		8.774	17.185	18.876	1.00 64.09)			N
	ATOM	4224	CA	CYS A 269		8.045	16.373	19.822	1.00 64.62				С
40	MOTA	4226	CB	CYS A 269		8.506	16.794	21.203	1.00 66.33				С
40	MOTA		SG	CYS A 269		10.286	17.212	21.240	1.00 69.02				S
	MOTA	4229		CYS A 269		6.523	16.452	19.735	1.00 64.55				С
	MOTA	4230	C	CYS A 269		5.943	17.350	19.089	1.00 67.99				0
	ATOM	4231	0	TRP A 270		5.899		20.395					N
4.5	MOTA	4232	N			4.444	15.334	20.512					С
45	MOTA		CA	TRP A 270			14.554						, C
	ATOM	4236	CB	TRP A 270		3.764	15.143		1.00 58.6			-	C
	MOTA	4239	CG	TRP.A 270		3.867	16.067						C
	MOTA	4240		TRP A 270									N
	MOTA	4242		TRP A 270		3.452	16.344						C
50	ATOM	.4244		2 TRP A 270		4.562					•		Ċ
. 1	MOTA	4245		2 TRP A 270		4.848							č
	MOTA	4246		3 TRP A 270		5.948							√,Ĉ
	MOTA	4248		3 TRP A 270		6.708						-	
	ATOM	4250	. CH	2 TRP A 270		6.395					•		C
55	ATOM	4252		2 TRP A 270		5.331							C
	ATOM	4254		TRP A 270		4.288							· C
	ATOM	4255	0 -	TRP A 270		5.212	13.830						0
	ATOM	4256		GLN A 271		3.112	14.664						N
	MOTA	4258		GLN A 271		2.891		23.791					C
60	ATOM	4260				1.547		24.328					C
JU	ATOM	4263				1.117		23.773	1.00 65.3	3			С
	ATOM	1200											

_	7.0004	40.00	CD (GLN A 271		1.086	16.093	22.229	1.00	63.95			C	;
5	ATOM	4266		GLN A 271		0.909	15.057	21.559		70.15			C)
	ATOM	4267		GLN A 271		1.256	17.287	21.674		54.26	,		N	-
	ATOM	4268		GLN A 271		2.931	12.731	23.697		56.78			C	3
	ATOM	4271		GLN A 271		2.634	12.186	22.647		57.25			C	
10	ATOM ·	4272		ALA A 272		3.274	12.068	24.774		55.14			ŀ	1
10	MOTA	4273		ALA A 272		3.457	10.637	24.671		58.98			(3
	MOTA	4275		ALA A 272		3.430	9.985	26.025		59.97			C	
	MOTA	4277		ALA A 272		2.422	10.009	23.754		59.71			(
	MOTA	4281		ALA A 272 ALA A 272		1.365	10.587	23.482		57.10			()
1.5	ATOM	4282		GLY A 273		2.782	8.821	23.271		62.02			ì	N
15	ATOM-	4283		GLY A 273		1.952	7.965	22.431		59.67				С
	ATOM	4285		GLY A 273		0.981	8.622			58.98		1	•	C
	MOTA	4288 4289		GLY A 273		0.009	7.967	21.115		61.66	٠		(0
	ATOM	4299		THR A 274		1.243	9.878	21.113		57.29			1	N
20	ATOM	4292		THR A 274		0.351	10.661	20.258		57.22				С
20	ATOM ATOM	4294		THR A 274		-0.108	11.911	21.023		63.52			. (С
	ATOM	4296		THR A 274		1.035	12.634	21.513	1.00	63.82				0
	ATOM	4298		THR A 274		-0.897	11.537	22.291	1.00	65.12				С
	MOTA	4302		THR A 274		0.994	11.128	18.943		54.80.				С
25	ATOM	4303		THR A 274		0.493	12.032	18.256	1.00	49.79				0
23	ATOM	4304	-	THR A 275		2.104	10.534	18.560	1.00	50.99				N
	ATOM	4306		THR A 275		2.712	11.010	17.345		50.86				С
	ATOM	4308		THR A 275		4.033	10.303	17.107		53.40				С
	ATOM	4310		THR A 275		4.793	10.248	18.331		53.69				0
30	ATOM	4312	CG2	THR A 275		4.901	11.074	16.111		48.79				С
	MOTA	4316	С	THR A 275.		1.736	10.679	16.226		52.73				C
	MOTA	4317	0	THR A 275		1.230	9.560	16.129		55.77				0
	MOTA	4318	N	PRO A 276	•	1.456	11.656	15.399		48.39				N C
	MOTA	4319	CA	PRO A 276		0.602	11.493	14:226		50.13				c
35	MOTA	4321	CB	PRO A 276		0.223	12.950			50.02 50.60				c
	MOTA	4324	CG	PRO A 276		1.513	13.620	14.213		53.12				č
	MOTA	4327	•	PRO A 276		1.877	13.055	15.554 12.974		42.85				Ċ.
	MOTA	4330	С	PRO A 276		1.265 1.501	10.862 11.537	11.980		39.08				o.
40	MOTA	4331	0	PRO A 276		1.527	9.567			46.18				N
40	ATOM	4332	N CZ	TRP A 277 TRP A 277		2.246	8.919	11.879		46.30				С
	ATOM	4334	CA	TRP A 277		2.339	7.449	12.146		41.35				С
	ATOM	4336	CB CG	TRP A 277		3.154	7.098	13.355		41.81				С
	ATOM	4339	CD1			2.696	6.545	14.489		45.45				С
45	MOTA MOTA	4340 4342	NE1			3.726	6.346	15.376	1.00	46.12				N
43	ATOM	4344		TRP A 277		4.886	6.784	14.809	1.00	40.67			Ţ,	С
• •	ATOM	4345		TRP A 277		4.565	7.263	13.538	1.00	42.28				С
	ATOM	.4346		TRP A 277		5.596	7.775	12.752	1.Ò0	45.83				С
	ATOM	4348		TRP A 277		6.872	7.785	13.257	1.00	41.25				С
50	ATOM	4350		TRP A 277		7.153	7.296	14.526	1.00	37.21				С
	ATOM	4352		TRP A 277		.6.185	6.798	15.316	1.00	40.09			•	С
:	MOTA	4354	C	TRP A 277		1.603	9.129	10.492		51.02				С
	ATOM		ō	TRP A 277		2.252	9.510	9.497		55.36				0
	ATOM	4356	N	ASN A 278		0.311	8.883	10.450		51.19		-	•	N
55	MOTA	4358	CA	ASN A 278		-0.467	9.067			46.14				C
:	ATOM	4360	СВ	ASN A 278		-1.925	8.947	9.660		51.01				С
•	ATOM	4363	CG	ASN A 278		-2,446		10.318		53.16			•	С
	ATOM	4364	OD1	ASN A 278		-2.406				56.07				0
	MOTA	4365	ND2	ASN A 278		-2.929		11.540		43.67				N
60	ATOM	4368	С	ASN A 278	•	-0.250				3 47.14				C
٠.	MOTA	4369	0	ASN A 278		-0.443	10.409	7.281	1.00	55.65				0

· 5	ATOM	4370	N	ILE A 279		0.154	11.459	9.136	1.00 4		•		N
-	ATOM	4372	CA	ILE A 279	4 .	0.262	12.647	8.283	1.00 4				C
	ATOM	4374	CB	ILE A 279		0.201	13.912	9.019	1.00 4				Ċ
	ATOM	4376	CG1	ILE A 279		1.508	14.087	9.747	1.00 4				C
	ATOM	4379		ILE A 279		1.810	15.503	10.041	1.00 4				С
10	ATOM	4383		ILE A 279		-1.078	13.936	9.940	1.00 4	0.98			С
10	ATOM	4387	C	ILE A 279		1.502	12.647	7.511	1.00 4	11.25			С
	ATOM	4388		ILE A 279		1.571	13.405	6.527	1.00 4	1.55			0
	MOTA	4389	N	PHE A 280		2.494	11.830	7.932	1.00 4	12.95			N
	ATOM	4391		PHE A 280		3.734	11.696	7.155	1.00 4	13.36			С
15	MOTA	4393	CB	PHE A 280		4.914	11.371	8.031	1.00 4	7.33	•		С
13	MOTA	4396	CG	PHE A 280		5.285	12.438	9.006	1.00 4	8.46			С
	ATOM	4397		PHE A 280		6.155	13.457	8.641	1.00 5				С
		4399		PHE A 280		6.512	14.437	9.555	1.00 5	55.06			C
	MOTA		CZ	PHE A 280		5.997	14.385	10.859	1.00 5				C
20	MOTA	4401		PHE A 280.		5.131	13.352	11.213	1.00 4				С
20	MOTA	4403		PHE A 280		4.791	12.401	10.296	1.00				С
	MOTA	4405		PHE A 280		3.596	10.572	6:116	1.00				С
	ATOM	4407	C			2.937	9.572	6.344	1.00				0
	ATOM	4408	0	PHE A 280		4.236	10.726	4.978	1.00				N
~~	MOTA	4409	N	PRO A 281		4.230	9.768	3.874	1.00				C
25	ATOM	4410	CA	PRO A 281		4.376	10.655	2.660	1.00				C
	ATOM .	4412	CB	PRO A 281		5.171	11.767	3.144	1.00				Č
	ATOM	4415	CG	PRO A 281			11.767	4.657	1.00		• •		Ċ
	MOTA	4418	CD	PRO A 281		5.116	8.679	3.868	1.00			٠,	c
	ATOM	4421	C .	PRO A 281		5.217		4.650	1.00				ŏ
30	ATOM	4422	0	PRO A 281		6.162	8.792	2.981	1.00				N ·
	ATOM	4423	N	VAL A 282		5.072		2.819	1.00				С
	ATOM .	4425	CA	VAL A 282		5.987	6.562		1.00				Ċ.
	ATOM	4427	CB	VAL A 282		5.215		2.365	1.00				C
	MOTA	4429		VAL A 282		4.205	4.818	3.377	1.00				Č
35	ATOM	4433		VAL A 282	٠.	4.500	5.499	1.028	1.00				Č
	MOTA	4437	C	VAL A 282		7.030	6.872	1.714	1.00				ŏ
	MOTA	4438	0	VAL A 282		6.797	7.738	0.873			•		Ŋ
	MOTA	4439	N	ILE A 283		8.156	6.136	1.705	1.00				C
	MOTA	4441	CA	ILE A 283		9.241	6.356	0.712	1.00 1.00				c
40	ATOM	4443	CB	ILE A 283		10.411	7.053	1.374					c
	ATOM	4445		ILE A 283		9.963	8.318	2.070					c
	ATOM	4448		ILE A 283		11.109	9.046	2.658	1.00				c
	MOTA	4452	CG2	ILE A 283		11.481	7.314	0.311		29.11			C
	ATOM	4456	С	ILE A 283		9.899	5.255	-0.053		41.40		•	o
45	ATOM	4457	0	ILE A 283		10.851	4.668	0.441		62.61			N
	MOTA	4458	N	SER A 284		9.483		-1.293	•	44.38			
	ATOM	4460	CA	SER A 284		9.856		-2.002		41.93			C
	MOTA	4462	CB	SER A 284		8.683	3.407	-2.819		42.78			C
	ATOM	4465	OG	SER A 284		7.555	3.197	-1.991		44.75			0
50	ATOM	4467	С	SER A 284		11.040	4.075	-2.897		44.34	•		Ç
	ATOM	4468	0	SER A 284		11.022	4.922	-3.788		46.55	• •		Ö
	MOTA	4469	N	LEU A 285		12.090	3.315	-2.656		41.54			N
	ATOM	4471	CA	LEU A 285		13.223	3.384	-3.521		37.02			С
	ATOM	4473	СВ	LEU A 285		14.491	3.276	-2.717	1.00	35.95	•		C
55	ATOM	4476	CG	LEU A 285		14.805	4.402	-1.704		38.01			С
	ATOM	4478		LEU A 285		16.196	4.144	-1.122	1.00	33.26			С
	ATOM	4482		LEU A 285		14.762	5.845	-2.251		33.22			С
•	ATOM	4486	C	LEU A 285		13.043	2.195	-4.451		38.43			С
	ATOM	4487	Ö	LEU A 285		12.880				43.06			0
60	ATOM	4488	N	TYR A 286		13.017	2.399			32.94			N
. 00		4490	CA	TYR A 286		12.855				39.45			С
	MOTA	4470	CA	11V W 500		22.000	1,202						

5	ATOM	4492	СВ	TYR A 286	12.115 1.611 -7.910 1.00 40.17	С
-	ATOM	4495	CG	TYR A 286	10.614 1.743 -7.827 1.00 37.69	С
	ATOM	4496		TYR A 286	10.025 2.618 -6.958 1.00 35.81	С
	ATOM	4498		TYR A 286	0.090 2.731 0.02.	C
	MOTA	4500	CZ	TYR A 286	7.894 1.996 -7.713 1.00 40.22	C
10	MOTA	4501	OH	TYR A 286	6.518 2.137 -7.632 1.00 32.05	0
10	MOTA	4503		TYR A 286	8.476 1.130 -8.584 1.00 39.77	С
		4505		TYR A 286	9.821 1.023 -8.648 1.00 35.63	С
	MOTA	4507	C	TYR A 286	14.207 0.832 -7.119 1.00 36.96	С
	MOTA	4508	0.	TYR A 286	14.990 1.654 -7.483 1.00 41.56	0
1.5	MOTA	4509	N .	LEU A 287	14.465 -0.461 -7.177 1.00 37.56	N
15	ATOM			LEU A 287	15.786 -0.941 -7.545 1.00 36.13	С
	ATOM	.4511	CA	LEU A 287	16.385 -1.695 -6.391 1.00 37.50	С
•	ATOM	4513	CB	LEU A 287	16.513 -1.001 -5.061 1.00 40.67	С
	ATOM	4516		LEU A 287	16.957 -2.079 -4.008 1.00 42.47	С
	MOTA	4518		LEU A 287	17.507 0.090 -5.144 1.00 37.99	C
20	MOTA	4522			15.760 -1.869 -8.700 1.00 32.81	С
	MOTA	4526	C	LEU A 287	14.789 -2.561 -8.889 1.00 42.24	0
	MOTA	4527	0	LEU A 287	16.849 -1.897 -9.447 1.00 37.48	N
	MOTA	4528	N	MET A 288	17.040 -2.777 -10.632 1.00 43.22	С
	MOTA	4530	CA	MET A 288	11 240 1 00 40 10	С
25 ·	MOTA	4532	CB	MET A 288	18.349 -2.356 -11.349 1.00 49.16 19.046 -3.419 -12.208 1.00 53.21	С
-	MOTA	4535	CG	MET A 288	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	S
	MOTA	4538	SD	MET A 288		C
	MOTA	4539	CE	MET A 288		C
	MOTA	4543	С	MET A 288		0
30	MOTA	4544	0	MET A 288	100 10 57	N
	MOTA	4545	N	GLY A 289		С
	MOTA	4547	CA	GLY A 289		Č
	MOTA	4550	C	GLY A 289	# · · · · · · · · · · · · · · · · · · ·	0
	ATOM-	4551	0	GLY A 289		N
-35	MOTA	4552	N	GLU A 290	100 00 00	C
	MOTA	4554	CA	GLU A 290	10.552	Č
	MOTA	4556	CB	GLU A 290	201000	č
	ATOM	4559	CG	GLU A 290	13.031	c
	MOTA	4562	CD	GLU A 290	10.001 11.001	Ö
40	ATOM	4563		GLU A 290	13.300	ŏ
	MOTA	4564	OE2	GLU A 290	21.142 -11.741 -9.471 1.00 55.78	č
	ATOM'	4565	С	GLU A 290	17.928 -9.808 -13.091 1.00 63.07	ö
	MOTA	4566	0	GLU A 290	18.755 -10.232 -13.887 1.00 67.93	N
	MOTA	4567	N	VAL A 291	16.643 -9.655 -13.398 1.00 65.43	C
45	ATOM	4569	CA	VAL A 291	16.189 -9.910 -14.769 1.00 66.54	č
	MOTA	4571	CB	VAL A 291	14.926 -10.790 -14.824 1.00 64.54	c
	MOTA	4573	CG1	VAL A 291	14.666 -11.196 -16.218 1.00 66.22	C
	MOTA	4577	··CG2	2 VAL A 291	15.116 -12.044 -14.013 1.00 66.62	. c
	ATOM	4581	С	VAL A 291	16.027 -8.615 -15.607 1.00 64.98	
50	ATOM	4582	0	VAL A 291	15.564 -7.590 -15.135 1.00 67.86	0
-	MOTA	4583	N ·	THR A 292	16.432 -8.687 -16.862 1.00 64.83	N
	ATOM	4585	CA	THR A 292	16.387 -7.554 -17.776 1.00 67.55	C
	ATOM	4587		THR A 292	16.783 -8.068 -19.139 1.00 69.56	C
	ATOM	4589		1 THR A 292	17.890 -8.965 -18.992 1.00 74.68	0
55	MOTA	4591		2 THR A 292	17.325 -6.980 -19.982 1.00 70.93	. С
"		4595	C	THR A 292	15.015 -6.878 -17.870 1.00 67.32	. С
	MOTA	4596		THR A 292	14.002 -7.532 -18.098 1.00 64.26	0
	ATOM	4597	N	GLN A 293	14.989 -5.562 -17.705 1.00 65.20	N
	MOTA	4599			13.735 -4.852 -17.700 1.00 65.67	С
C O	MOTA				7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	С
60	MOTA	4601			5 010 10 070 1:00 00 00	С
	MOTA	4604	ÇG	ODN R 233	40.5.	

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                       ARG A 297
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                       ARG A 297
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                                                                                     С
                       ARG A 297
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40
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                                                               1.00 45.80
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             4685 ·
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                       ILE A 298
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                                                                                      C
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5	ATOM ·	4719	N	ILE A 3	300		9.561	2.371	2.818		45.04		N
•	ATOM	4721		ILE A 3		. •	9.712	2.602	4.257		43.86		C .
•	MOTA	4723	CB	ILE A 3	300		11.112	3.118	4.717		43.97		C
	ATOM	4725	CG1	ILE A 3	300		11.584	4.378	4.011		45.01		C
	MOTA	4728	CD1	ILE A 3	300		12.548	5.177	4.939		40.08		C ·
10	MOTA	4732	CG2	ILE A 3	300		12.167	2.091	4.499		47.96		C
	MOTA	4736	С	ILE A 3	300		8.619	3.494	4.769		43.59		С
•	MOTA	4737	0	ILE A 3	300		7.878	4.094	4.001		44.78		0
	MOTA	4738	N	LEU A 3	301		8.538	3.556	6.089		41.32		Ŋ
	MOTA	4740	CA	LEU A	301		7.515	4.294	6.798		39.77		Ċ
15	ATOM	4742	CB	LEU A 3	301		6.837	3.315	7.759		34.77		.C.
	MOTA	4745	CG	LEU A	301		6.052	2.205	7.119		30.44		C
	ATOM	4747	CD1	LEU A	301		5.467	1.524	8.188		30.86		C .
	ATOM	4751	CD2	LEU A	301		4.968	2.698	6.252		34.38		C,
•	ATOM	4755	С	LEU A	301 .		8.106	5.431	7.632		39.51		C
20	ATOM	4756	0	LEU A			9.292	5.472	7.850		44.43		0
	MOTA	4757	N	PRO A	302		7.286	6.338	8.142		38.79		N
	MOTA	4758	CA	PRO A	302		7.819	7.393	9.001		36.78		C
	MOTA	4760	CB	PRO A	302		6.590	8.187	9.424		37.00		C
	ATOM	4763	CĠ	PRO A	302		5.410	7.604	8.714		36.36		C
25	MOTA	4766	CD	PRO A	302·		5.832	6.424	7.958		36.66		C
	MOTA	4769	С	PRO A	302		8.510	6.797	10.226		38.02		C
	MOTA	4770	0	PRO A			9.516	7.327	10.642		33.13		0
	MOTA	4771	N	GLN A	303		7.995	5.719	10.811		38.55		N
	MOTA	4773	CA	GLN A	303		8.699	5.129	11.945		36.57		C
30	ATOM -	4775	CB	GLN A	303		8.003	3.902	12.457		35.69		C
-	ATOM	4778	CG	GLN A			6.751		13.195		42.25		C.
	MOTA	4781	CD	GLN A		•	••••	4.274	12.297		34.75		C O
•	MOTA	4782		GLN A			5.772	4.591	11.130		46.30		N
٠	ATOM	4783	NE2	GLN A			4.416	4.026	12.820		42.67		C
35	MOTA .	4786	С	GLN A		•	10.113		11.588		42.43		0
	MOTA	4787	0	GLN A			10.807	4.115	12.404		44.66		N
•	ATOM	4788	N.	GLN A			10.554	4.872	10.373		44.05	•	C
	MOTA	4790	CA	GLN A			11.919	4.525	10.089		43.84 44.50		C
	MOTA	4792	CB	GLN A			12.025	3.506	8.939		44.50		C
40	MOTA	4795	CG	GLN A			11.789	. 2.069	9.464		41.50		č
	ATOM	4798	CD	GLN A		•	10.436	1.517	9.204		46.70		ŏ
	MOTA	4799		GLN A			9.915	0.808	10.039 8.050		43.88		N
	MOTA	4800		GLN A			9,849	1.830			43.47	•	c
4-	MOTA	4803	C	GLN A			12.735	5.769	9.864 10.460		57.31		ŏ
45	ATOM	4804	0	GLN A			13.806	5.890	9.056		43.84		N
	MOTA	4805	N	TYR A			12.253	6.709	8.789		42.11		c
	MOTA	4807	CA	TYR A			13.030	7.931 8.542	7.383		42.55		Č
	MOTA	4809	CB				12.741	9.026	7.065		38.35		c
	MOTA	4812	CG	TYR A			11.329		7.553		39.92		c
. 50	MOTA	4813		TYR A		•	10.846	10.230 10.679	7.245		38.06		č
	MOTA	4815		TYR A			9.579				44.35		Č
	MOTA	4817	CZ	TYR A			8.745	9.931	. 6.432		47.26		ŏ
•	MOTA		OH	TYR A			7.445	10.380					Ç.
ے نے	MOTA	4820		TYR A			9.206	8.737	5.934		1 30 60	• •	Ċ
55	ATOM	4822		TYR A			10.502	8.296	6.252 9.901		39.60 342.17		c.
,	MOTA	4824	С	TYR A			12.920	8.991			47.00		ŏ
	ATOM	4825	0	TYR A			13.587	10.034	9.828 10.910		38.60		N
	ATOM	4826	N	LEU A			12.096	8.727			2 42.86		·C
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60	MOTA	4830	CB	LEU A			10.473	9.989	12.345				c
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	ATOM	5056	CG	LYS	A 321	•	17.182	15.141	15.141	1.00 53.31		2
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10	MOTA	5062			A 321		19.429	16.349	15.512	1.00 55.80	(
10	ATOM	5065		LYS	A 321		20.917	16.178	15.790	1.00 57.93		1
	MOTA	5069			A 321		14.857	13.255	13.163	1.00 43.54		3
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	MOTA	5071	N		A 322		14.947	14.097.	12.161	1.00 41.25		N.
15	MOTA	5073			A 322		14.655	13.750	10.791	1.00 43.43		C
13	ATOM	5075	CB		A 322		14.199	15.061	10.075	1.00 45.65	. (C
	ATOM	5078	CG.		A 322		13.807	14.910	8.629	1.00 41.86		С
	MOTA				A 322		12.758	14.134	8.257	1.00 41.79		С
		5081			A 322		12.427	14.000	6.960	1.00 37.29	. •	C.
20	MOTA	5083	CZ		A 322		13.125	14.653	5.982	1.00 40.05		C
20	ATOM		CES		A 322		14.158	15.436	6.310	1.00 42.54		С
	ATOM	5085			A 322		14.509	15.566	7.642	1.00 46.49		С
	MOTA	5087			A 322		15.961	13.138	10.239	1.00 48.97	1	С
	MOTA	5089	C		A 322		16.981	13.817	10.014	1.00 48.91		0
	MOTA	5090	0				15.922	11.831	10.036	1.00-42.08		N
25	ATOM	5091	N		A 323		17.072	11.115	9.597	1.00 39.45		С
	ATOM	5093	CA		A 323		17.072	9.753	10.228	1.00 38.16		С
	MOTA	5095	CB		A 323			11.012	8.047	1.00 42.70		С
	MOTA	5099			A 323		17.297	10.006	7.562	1.00 40.41		0
••	ATOM	5100			A 323		17.863	12.027	7.268	1.00 39.06		N
30	ATOM	5101	N		A 324		16.914	11.971	5.799			C
	MOTA	5103	CA		A 324		17.177	12.049	4.976	1.00 35.33		Ċ
	MOTA	5105	CB		A 324		15.911		5.158	1.00 41.82		c
	MOTA	5107			A 324		15.063	10.826	4.283	1.00 45.15		Č
	ATOM	5110			A 324		13.800	10.854	3.553	1.00 39.72		c
35	ATOM	5114			A 324		16.241	12.092	5.453	1.00 41.45		c
	ATOM	5118	C		: A 324		18.000	13.179	5.571	1.00 47.75		o.
	MOTA	5119	0		A 324		17.491	14.268	5.011	1.00 47.73		N
	MOTA	5120	N		A 32!		19.244	13.022		1.00 47.83		C
	MOTA	5122	CA		A 32		20.148			1.00 47.03		Č.
40	MOTA	5124	CB		A 32		21.194	14.129	5.977	1.00 51.02		Ō
	MOTA	5127	OG		R A 32		21.991	12.978	5.786	1.00 44.39		C
	ATOM	5129	С		R A 32		20.831	14.230	3.573	1.00 44.39		o
	MOTA	5130	0		R A 32		20.699	13.316	2.780			N
	MOTA	5131	N		1 A 32		21.579	15.286	3.320	1.00 49.08		C
45	MOTA	5133	CA		1 A 32		22.095	15.527	1.954	1.00 50.41 1.00 50.65		č
	MOTA	5135	CB		1 A 32		21.980	17.004	1.575			c
	MOTA	5138	CG		1 A 32		22.818	17.900	2.410	1.00 59.27		C
	ATOM	5141	CD		N A 32		22.308	19.336	2.379	1.00 69.60		
	ATOM	5142	OE1	. GL1	N A 32	6 [22.805		1.608	1.00 81.67		O.
50	MOTA	5143	NE2	GLi	N A 32	6	21.315	19.636		1.00 74.53		N
	ATOM	5146	C.	GL	N A 32	6 ·	23.522	15.036		1.00 47.73		C
	MOTA	5147	Ο.	GLi	N A 32	6	24.139			1.00 39.28		0
	ATOM	5148	N	SEI	R A 32	7	24.036	14.838	0.616	1.00 50.50		N
	ATOM	5150	CA ·		R A 32		25.349			1.00 48.29		С
55	ATOM	5152	СВ		R A 32		25.170			1.00 50.33		C
ور	ATOM	5155	OG		R A 32		26.109			1.00 44.83		0
	ATOM	5157			R A 32		26.057		-0.934	1.00 54.98		C
	MOTA	5158			R A 32		25.440		-2.005			0
	ATOM	5159			R A 32		27.375			1.00 58.53		N
60	ATOM	5161			R A 32		28.228			1.00 59.21		С
00	MOTA	5163			R A 32		29.294			1.00 59.74		С
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5	MOTA	5166	OG	SER A 328		30.068	15.264	-0.446		58.39			O C
	MOTA	5168	С	SER A 328	-		13.650		1.00	63.61			o
	MOTA	5169	0	SER A 328		29.458	13.656	-3.630	1.00				N
	ATOM	5170	N	THR A 329		28.861	12.588	-1.696	1.00				C
	ATOM	5172	CA	THR A 329		29.372	11.305	-2.132	1.00			•	
10	ATOM	5174	СВ	THR A 329		30.254	10.683	-1.073		59.15			C
	ATOM	5176	OG1	THR A 329		29.635	10.794	0.212		56.80			0.
	ATOM	5178	CG2	THR A 329		31.542		-0.972		61.68			C
	ATOM	5182	С	THR A 329		28.280	10.328	-2.543		55.97			C
	ATOM	5183	0 ′	THR A 329		28.473	9.113	-2.470		61.73			0
15	ATOM	5184	N	GLY A 330	•	27.131		-2.965		52.78			N.
	ATOM	5186	CA	GLY A 330		26.102	9.994	-3.558		47.81			С
	ATOM	5189	С	GLY A 330	٤,	25.072	9.508	-2.565		40.66		•	C.
	ATOM	5190	0	GLY A 330		25.057	9.994	-1.446		41.70			0
4	ATOM	5191	N	-THR- A 331		24.242	8.545	-2.962		37.29			N
20	ATOM	5193	.CA	THR A 331		23.170	8.072	-2.094		37.86			C
20	MOTA	5195	CB	THR A 331		22.068	7.313	-2.904		39,26		•	С
	ATOM	5197		THR A 331		21.479	8.139	-3.916		39.31			0
	ATOM	5199		THR A 331		20.888	7.049	-2.051		42.31			С
	MOTA	5203	С	THR A 331		23.756	7.124	-1.078		39.73			С
25	MOTA	5204	o i	THR A 331		24.660	6.353	-1.407		44.56			0
.23	ATOM	5205	N	VAL A 332		23.258	7.178	0.154		40.26			N
	ATOM	5207	CA	VAL A 332		23.641	6.187	1.152		35.90			C ·
	ATOM	5209	СВ	VAL A 332		24.604	6.690	2.229		40.57			С
	ATOM	5211		VAL A 332		24.912	5.525	3.187		39.73			С
30	ATOM	5215		VAL A 332		25.881	7.177	1.612		41.22			С
30	ATOM .	5219	С	VAL A 332		22.424	5.582	1.853		42.39			С
	ATOM	5220	ō	VAL A 332		21.729	6.293	2.599		41.60			0.
	ATOM	5221	N	MET A 333		22.203	4.285	1.594		37.82			N
	ATOM	5223		MET A 333		21.117	3.471	2.170		36.93			С
35	MOTA	5225	СВ			20.723	2.317	1.246		37.72		•	С
33	ATOM	5228	CG	MET A 333		20.166	2.782	-0.085		41.56			C
	MOTA	5231	SD	MET A 333		19.579	1.455	-1.132		50.56			S
	MOTA	5232	CE	MET A 333		18.013	1.284	-0:388		55.20			C
	ATOM	5236	C	MET A 333		21.588	2.919	3.503		41.46			С
40	ATOM	5237	0	MET A 333		22.205	1.777	3.611		39.46			0
	MOTA	5238	N	GLY A 334		21.291	3.762	4.508		40.49			N
	ATOM		- CA	GLY A 334		21.812	3.648	5.846		38.05			С
	ATOM	5243	С	GLY A 334		20.941	2.902	6.789		38.82			С
	ATOM	5244	0	GLY A 334		19.921	2.335	. 6.417		44.15			0
45	ATOM	5245	N	ALA A 335		21.359	2.914	. 8.045		38.69			N
. •-	ATOM	5247	CA			20.658	2.169	9.044	•	38,89			C
	MOTA	5249	СВ			21.021	2.632	10.403		39.90		•	C
	ATOM	5253				19.193	2.369	8.825		42.45			C
•	ATOM	5254		ALA A 335		18.353	1.432	8.827		41.48			0
50	ATOM	5255	N	VAL A 336		18.830		8.611		43.44			N
30	ATOM	5257	CA			17.425		8.643		46.66			С
	ATOM	5259	СВ			16.973		8.808	1.00	49.40			C
	ATOM	5261		1 VAL A 336		17.623				55.39			С
	ATOM	5265		2 VAL A 336		17.340				52.52			С
55		5269		VAL A 336		16.921			1.00	46.80		-	С
23	MOTA	5270		VAL A 336		16.221	_		1.00	0 48.30			0
	ATOM	5270	N	ILE A 337	•	17.318				0 45.47			N
	ATOM	5271				16.677				0 36.74			С
	ATOM	5275				17.298				0 39.78			С
60	MOTA	5277		1 ILE A 337		17.151				0 36.27			С
60	MOTA			11 ILE A 337		15.779				0 43.14			С
	ATOM	5280	CL	,		10.77							

	•											
5	MOTA	5284	CG2	ILE A		_ 16.67i		2.978	1.00 34.84	•		C
	MOTA	5288	С	ILE A	337	16.885		5.806	1.00 39.51	- " .	-	С
	MOTA	5289	0	ILE A	337	16.013	-0.096	5.623	1.00 35.70			О
	MOTA	5290	N	MET A	338	18.031	0.511	6.397	1.00 38.60			N
	ATOM	5292	CA	MET A	338	18.215	-0.928	6.662	1.00 39.01			С
10	MOTA	5294	CB	MET A	338	19.673	-1.259	7.028	1.00 37.15			C
	MOTA	5297	CG	MET A	338	20.587	-1.321	5.812	1.00 38.15			С
	ATOM	5300	SD	MET P		22.320		6.100	1.00 49.00			S
•	ATOM	5301	CE	MET A		22.236	-3.500	6.563	1.00 47.85		• .	С
	ATOM	5305	C	MET F		17.197		7.680	1.00 36.06			С
15	ATOM	5306	ō	MET A		16.768		7.615	1.00 40.65			0
13	ATOM	5307	N .	GLU A		16.780		8.610	1.00 43.64			N
	ATOM	5309	CA	GLU A		15.981		9.755	1.00 43.34			С
	ATOM	5311	CB	GLU F		15.922		10.811	1.00 44.54		•	С
•	ATOM	5314	CG ·	GLU F		16.905	•	11.984	1.00 50.03			С
20	ATOM	5317	CD	GLU I		17.134		12.854	1.00 50.19			С
20	MOTA	5318		GLU F		18.297			1.00 50.60			0
	ATOM	5319		GLU A		16.170		13.133	1.00 52.29			0
	ATOM	5320	C	GLU A		14.593		9.375	1.00 44.44			С
	ATOM	5321	Ö	GLU A		13.825		10.235	1.00 48.83			0
25	ATOM	5322	Ŋ	GLY A		14.25		8.096	1.00 37.01			N
23	ATOM	5324	CA	GLY A		13.003		7.664	1.00 35.04			Ċ
	ATOM	5327	C		340	13.074		7:035	1.00 37.57			С
	ATOM	5328	o	GLY A		12.06		6.954	1.00 30.82			0
	MOTA	5329	N		341	14.25		6.584	1.00 36.28			N
30 -	ATOM	5331	CA	PHE A		14.28		5.860	1.00 37.94	•	•	С
30 .	ATOM	5333	CB.		341	14.549		4.467	1.00 35.78			C
	ATOM	5336	CG		A 341	13.72			1.00 36.57			С
	ATOM	5337		PHE A		14.14		4.214	1.00 42.48			С
	ATOM	5339		PHE A		13.36		3.810	1.00 45.68	-		. C
35	ATOM	5341	CZ		A 341	12.16		3.237	1.00 43.50			С
33	MOTA	5343		PHE A		11.73		3.058	1.00 39.45			С
	ATOM	5345		PHE A		12.49		3.451	1.00 39.09			С
	ATOM	5347	C		A 341	15.28		6.323	1.00 37.29			С
	ATOM	5348	ō		A 341	16.01		7.200	1.00 41.19			0
40	ATOM	5349	N		A 342	15.29		5.745	1.00 38.28	•		N
40	ATOM	5351	CA		A 342	16.29		6.079	1.00 39.65		•	C
	ATOM	5353	CB		A 342	15.71		6.073	1.00 40.40			. C
	ATOM	5356	CG		A 342		4 -10.890	6.407	1.00 41.95			С
	ATOM	5357		TYR			5 -10.727		1.00 43.94			С
45	ATOM	5359			A 342		8 -11.731		1.00 48.72			. C
1.5	ATOM	5361	CZ		A 342		5 -12.947		1.00 49.33			С
	ATOM	5362	OH		A 342		9 -13.922		1.00 51.44			0
	ATOM	5364			A 342		2 -13.159		1 .			. C
	ATOM	5366		TYR			3 -12.122		1.00 47.27			С
50	ATOM	5368	C		A 342	17.11			1.00 36.83			С
, 30	MOTA	5369	Ö		A 342	16.56			1.00 38.58			0
	ATOM	5370	N		A. 343				1,00 32.01			N
	ATOM	5372	CA		A 343	19.20						С
	ATOM	5374	CB		A 343	20.07				•		С
55	ATOM	5374			A 343	•					•	C
33		5380			A 343					•		C
	ATOM	5384	C.		A 343				1.00 41.31			Č
	MOTA		0		A 343							ŏ
	ATOM	5385 5386			A 344							N
60	MOTA	5386	N		A 344		2 -10.337					c
vv	MOTA	5388	CA				0 -11.348					č
	MOTA	5390	CB	VAL	A 344	20.42	U -11.348	1.500	1.00 33.00			_

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5	MOTA	5392	CG1	VAL A 344	21.253 -12	2.622	1.272	1.00				C
7	MOTA	5396 -	CG2	VAL A 344	 -19.17311	1.671	2.320	1.00			-	C
	ATOM		С	VAL A 344	22.433 -10	0.004	1.360	1.00				С
	ATOM		ō	VAL A 344	22.298 -	9.878	0.166	1.00	36.99			0
		•	N .	PHE A 345		9.871	1.945	1.00	36.90			N
10	ATOM			PHE A 345		9.592	1.141	1.00	36.18			С
10	ATOM		CA	PHE A 345		8.841	1.954	1.00				С
	MOTA		CB	PHE A 345		7.408	2.249	1.00			•	С
	ATOM		CG			6.348	1.501	1.00				С
	MOTA			PHE A 345		5.139	1.797	1.00				С
	MOTA			PHE A 345			2.850	1.00				С
15	ATOM		CZ	PHE A 345		4.914	3.581	1.00				c
	ATOM	5416		PHE A 345		5.924		1.00				Ċ
	ATOM	5418	CD2	PHE A 345	24.597 -		3.279	1.00				c
	ATOM	5420	C.	PHE A 345	25.443 -1		0.522					o
•	MOTA	5421	0	PHE A 345	26.486 -1		0.958	1.00				
20	ATOM	5422	N	ASP A 346	24.785 -1		-0.525	1.00				N
20	MOTA	5424	CA	ASP A 346	25.157 -1	2.498	-1.257	1.00				С
	ATOM	5426	СВ	ASP A 346	23.865 -1	2.940	-1.938	1.00				С
	ATOM	5429	CG	ASP A 346	23.993 -1		-2.742		44.26			С
	ATOM	5430		ASP A 346	25.122 -1		-2.972	1.00	49.09			´ Q
26		5431		ASP A 346	22.961 -1		-3.196	1.00	44.53			0
25	MOTA			ASP A 346	26.310 -1		-2.247	1.00	37.90			С
	MOTA	5432	С	ASP A 346	26.156 -1		-3.481		32.28			0
	MOTA	5433	0	ARG A 347	27.498 -1		-1.659		40.60			N
	MOTA	5434	N		28.764 -1		-2.385		37.22			С
	MOTA	5436	CA	ARG A 347	29.896 -1		-1.348	1.00				C
30	MOTA	5438	CB		29.896 -1		-0.457		34.79			С
	MOTA	5441	CG	ARG A 347					35.83			C
	ATOM	5444	CD	ARG A 347	30.720 -1				46.81			N
	MOTA	5447"	NE	ARG A 347	32.086 -1		0.381		48.24			C
	MOTA	5449	CZ	ARG A 347	33.161 -1		0.700					N
35	MOTA	5450		ARG A 347	33.029 -		1.397		55.18			N
	MOTA	5453	NH2	ARG A 347	34.372 -1		0.317		45.55			· C
	MOTA	5456	С	ARG A 347	28.920 -		-3.429		36.71	•		
	MOTA	5457	0	ARG A 347	29.227 -		-4.573		45.36			0
	MOTA	5458	N	ALA A 348	28.699 -	14.501	-3.041		42.24			N
40	ATOM	5460	·CA	ALA A 348	28.835 -3		-3.960		46.74			C
	ATOM	5462	CB	ALA A 348	28.168 -	16.883	-3.369		49.53			C
	MOTA	5466	С	ALA A 348	28.256 -	15.440	-5.301		43.78			. C
	ATOM	5467	0	ALA A 348	28.804 -	15.893	-6.279	1.00	51.15			0
	ATOM	5468	N	ARG A 349	27.114 -	14.772	-5.347		50.73			N
45	MOTA	5470	CA	ARG A 349	26.435 -		-6.606	1.00	45.15			С
73.	ATOM	5472	ĊВ	ARG A 349	25.008 -	15.048	-6.522	1.00	46.17			С
		5475	CG	ARG A 349	25.021 -		-6.566	1.00	50.92			С
	ATOM	5478	CD	ARG A 349	23.678 -		-6.431		56.96			С
	MOTA			ARG A 349	22.731 -	17.167	-7.546	1.00	58.75		•	N
	MOTA	5481	NE		21.525 -	17.757	-7.576		59.56	•		С
50	MOTA	5483	CZ	ARG A 349	21.140 -	19 544	-6.575		56.83			N
	ATOM	5484		1 ARG A 349	21.140 -	17 676	-8.596		57.83	:		N
	. ATOM	5487		2 ARG A 349	20.699 -	12 000			46.61			C
	ATOM	5490	С	ARG A 349	26.515 -	13.088	-7.031			•		ŏ
	ATOM	5491	0	ARG A 349	26.054 -	12.752			48.78			N
55	ATOM	5492	N	LYS A 350	27.108 -	12.227	-6.198		43.49			
	ATOM	5494	CA	LYS A 350	27.257 -	10.824	-6.565		39.81			C
	ATOM	5496	CB	LYS A 350	27.981 -		-7.901		42.63			C
	ATOM	5499	CG	LYS A 350		-9.252	-8.257		54.21			C
	ATOM	5502	CD			-9.124	-9.427		58.86			C
60	ATOM	5505	CE			-7.616	-9.867		62.75			C
50	ATOM	5508	NZ		30.583	-7.261	-10.973	1.00	61.28			N
	MION	5550										

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1.00 42.26
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                      LYS A 350
    MOTA
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                       LYS A 350 ...
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                   CD
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                   NH1 ARG A 351
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                                                                1.00 34.43
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            5536
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     MOTA
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                       ARG A 351
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                                       22.562
                       ILE A 352
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                                                                                      С
                       ILE A 352
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                                                        -2.397
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                       ILE A 352
                                                        -2.051
                                       22.232
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                   CB
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                   CG1 ILE A 352
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                                                        -2.019
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                                                        -2.366
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                   CD1 ILE A 352
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                                                                1.00 32.36
                      ILE A 352
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                       ILE A 352
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                       GLY A 353
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                   С
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                   CA
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     ATOM
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                                               -5.078
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                   CD1 PHE A 354
                                       17.323
             5572
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                   CE1. PHE A 354
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                                               -3.320
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                       PHE A 354
                                       18.742
             5576
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                                                                                       С
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                                                         0.571 1.00 27.61
             5578
                   CE2 PHE A 354
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                                                                                       С
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             5583
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                                                                                       N
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             5586
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                                                                1.00 28.36
             5588
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     MOTA
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                                                                1.00 31.09
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45
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                                                         3.860
                       VAL A 356
                                       10.912
             5594
                   Ν .
     MOTA
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                                                                                       C
                                                         4.958
                       VAL A 356
                                       10.326
                                                -7.206
             5596
                   CA
     ATOM
                                                -7.269
                                                                1.00 36.49
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                                        8.800
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                   CB
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                                        8.258
                   CG1 VAL A 356
                                                -6.199
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                                       8.253
                                                -7.092
                                                        . 3.695
                                                                1.00 35.72
50
                       VAL A 356
     MOTA
             5604
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                                                                1.00 41.52
                                                                                       C
                                                -7.852
                                                         6.243
                       VAL A 356
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             5608
                   С
                                                         6.331
                                                                1.00 37.93
                                                                                       0
                       VAL A 356
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                                                                1.00 43.38
                                                                                       N
                       SER A 357
                                      11.104
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                   N
                                                                                       C
                       SER A 357
                                       11.551
                                                -7.584
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             5612
                   CA
                                                          9.235
                                                                1.00 45.00
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                                                -6.514
                       SER A 357
                                       12.327
 55
                   CB
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             5614
                                                                                       0
                                       13.156
                                                -7.090
                                                        10.258
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                       SER A 357
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     MOTA
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                        SER A 357
                                       10.410
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                                                          9.314
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                                                -7.417
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                        ALA A 358
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      MOTA
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                                                                 1.00 47.19
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      MOTA
             5623
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                                                        11.270
                                                                 1.00 44.33
                       ALA A 358
      MOTA
             5625
                    CB
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5	ATOM	5629	C.	ALA A	358		9.858	-8.814	12.486	1.00	53.26			C
	MOTA	5630	0	ALA A		-	9.324	-9.302	13.472		58.72 · · ·			0
	ATOM	5631	N	CYS A	359		10.720	-7.790	12.540		54.45			N C
	MOTA	5633	CA	CYS A			10.962	-7.065	13.779		52.85			C
	ATOM .	5635	CB	CYS A			12.325	-7.455	14.429		55.72			S
10	MOTA	5638	SG	CYS A			13.911	-6.785	13.755		65.10 53.76			C
	ATOM	5639	С	CYS A			10.793	-5.543	13.583		60.53			ŏ
	MOTA	5640	0	CYS A			11.047	-4.789	14.519		45.54			И
	MOTA	5641	N	HIS A			10.332	-5.075	12.412		38.19			c
	MOTA	5643	CA		360 .		10.265	-3.631	12.161 10.655		31.06			č
15	MOTA	5645	CB	HIS A			10.274	-3.291	9.972		34.23			Ċ
	MOTA	5648	CG	HIS A		-		-3.409	9.566		43.85		•	N
	MOTA	5649		HIS A			8.422	-4.617 -4.425	8.979		30.40			C
	MOTA	5,651		HIS A			7.259		8.992		36.44			N
	MOTA	5653		HIS A			7.010	-2.475	9.607		29.91			С
20	ATOM	5655		HIS A			8.051 9.170	-2.820	12.921		41.87			Č.
	MOTA	5657	С	HIS A			8.085	-3.281	13.248		47.13			0
	MOTA	5658	0	HIS A		•	9.488	-1.576	13.194		36.30	•		N
-	MOTA	5659	N	VAL A			8.626	-0.768	13.971		36.06			С
٥٠	MOTA	5661	CA	VAL A			9.448	0.396	14.601		33.69			С
25	ATOM	5663	CB	VAL A			8.519	1.388	15.203		33.28			С
	ATOM	5665		VAL			10.371	-0.136	15.590		30.28			С
	ATOM	5669	C				7.498	-0.219	13.100		35.37			Ç
	ATOM -	5673 5674	0	VAL A			7.749	0.397	12.095		28.73			0
30	ATOM	5675	N	HIS A			6.262	-0.453	13.489	1.00	38.93			N
,30	ATOM	5677	CA		362			0.046		1.00	43.25			С
	ATOM	5679	CB	HIS F			4.939	-0.771	11.462	1.00	43.67			С
	ATOM	5682	CG	HIS A			4.555	-2.203	11.705		46.38			С
•	ATOM	5683		HIS A			5.479	-3.210	11.850	1.00	49.03			N
35	ATOM	5685		HIS A			4.855	-4.363	12.037		50.56			С
55	ATOM	5687		HIS A			3.558	-4.143	12.013		45.23		•	N
	ATOM	5689		HIS A			3.345	-2.799	11.810		51.21			C
	ATOM	5691	С	HIS A	A 362		3.831	0.124	13.587		44.78			С
	ATOM	5692	0	HIS A	A 362		3.871	-0.147	14.749		49.93			0
40	MOTA	5693	N	ASP A	A 363		2.704	0.524	13.028		48.91			N
	MOTA	5695	CA	ASP Z	A 363		1.412		13.729		48.67			C C
	ATOM	5697	CB	ASP I	A 363		0.779	1.835	13.601		48.80			c
•	MOTA	5700	CG		A 363		0.798	2.252	12.190		56.05			Ö
	MOTA	5701		L ASP			0.064	1.570	11.427		62.04			o
45	ATOM	5702	OD2	ASP			1.530	3.170	11.732		53.10			c
	MOTA	5703	С		A 363		0.583	-0.390		•	50.55			Ö
	MOTA	5704	0		A 363		1.082	-0.877	11.824		49.82			N
	ATOM	5705	N		A 364		-0.698		13.161		51.52			c
	MOTA	5707		GLU .				-1.526	12.443		50.07			č
50	MOTA	5709	CB		A 364		-2.705				54.11			č
	ATOM	5712	ÇG		A 364		-3.727	-0.871			56.03			.C
	MOTA	5715	CD		A 364		-5.070				0 64.46			0
	MOTA	5716		l GLU			-6.040	-0.598			76.03			Ö
	MOTA	5717		2 GLU			-5.182	-2.618			0 46.64			c
55	MOTA	5718	C		A 364		-1.989				0 47.66 0 47.48			. 0
	MOTA	.5719	0		A 364		-2.524	-1.783						N
	MOTA	5720	N		A 365		-1.799				0 41.55 0 44.15			. C
	MOTA	5722			A 365		-2.309				0 44.13			C
	ATOM	5724	CB		A 365		-2.603				0 42.04			č
60	ATOM	5727	CĠ		A 365		-3.640 -3.391				0 42.11			C
	MOTA	5728	CD	1 PHE	A 365		-3.331	3.047	14.140	1.0	. 30.14			-

5	ATOM	5730	CE1	PHE A	A 365		-4.332	3.195	13.033	1.00 43.1	7		С
•	ATOM	· 5732·	CZ	PHE A	A 365		-5.532	2.685	12.820	1.00 47.9			С
	MOTA	5734	CE2	PHE A	A 365		-5.793	2.006	11.673	1.00 50.5			C
	ATOM	5736	CD2	PHE A	A 365		-4.869	1.858	10.771	1.00 47.3	7		C
	MOTA	5738	С	PHE A	A 365		-1.462	0.662	8.321	1,00 46.29			C
10	MOTA	5739	0	PHE A	A 365		-2.031	0.487	7.227	1.00 49.3			0
	ATOM	5740	Ν .	ARG A	A 366		-0.143	0.745	8.428	1.00 42.8	j .		N
	MOTA	5742	CA	ARG Z	A 366		0.796	0.645	7.309	1.00 41.9	Ĺ		C
	MOTA	. 5744	CB	ARG A	A 366		1.398	1.997	6.985	1.00 40.9	6		С
	MOTA	5747	CG	ARG I	A 366		0.536	2.993	6.424	1.00 40.9			С
15	ATOM	5750	CD.	ARG A	A 366		1.341	4.073	5.811	1.00 40.8	3.	•	С
	ATOM	5753	NE	ARG A	A 366		1.839	4.979	6.843	1.00 40.9	7		N
•	ATOM	5755	CZ		A 366		1.893	6.275	6.661	1.00 40.9			С
	ATOM	5756	NH1	ARG A	A 366		1.476	6.743	5.493	1.00 36.3	6	•	N
•	MOTA	5759	NH2	ARG A	A 366		2.346	7.096	7.609	1.00 40.3	3.		N
20	ATOM	5762	С		A 366		2.061	-0.090	7.758	1.00 41.9	3		С
	ATOM	5763.	0		A 366		2.491	0.129	8.894	1.00 41.5	9		0
	MOTA	5764	N		A 367		2.677	-0.865	6.847	1.00 37.7	2		N
	ATOM	5766	CA	THR 2	A 367		3.839	-1.681	7.138	1.00 33.6	5		С
	ATOM	5768	ĊВ	THR I	A 367		3.469	-3.107	7.143	1.00 42.3	2		С
25	ATOM	5770	OG1	THR A	A 367		4.646	-3.854	6.891	1.00 43.8	4		0
	MOTA	5772	CG2	THR 2	A 367		2.528	-3.460	5.969	1.00 43.3			С
٠.	MOTA	5776	С	THR	A.367		4.827	-1.507	6.066	1.00 32.7	2		С
	ATOM	5777	0	THR .	A 367		4.465	-1.157	4.970	1.00 34.9	В	•	0
•	ATOM	5778	N		A 368		6.110	-1.702	6.359	1.00 39.9	2	•	N
30	ATOM	5780	CA		A 368		7.135	-1.504	5.307	1.00 40.5	0		С
-	ATOM	5782	CB	ALA .	A 368	•	8.485	-1.608	5.870	1.00 38.7	2		С
	ATOM	5786	С		A 368		6.910	-2.529	4.180	1.00 43.3	3		С
	ATOM	5787	0		A 368		6.181	-3.498	4.382	1.00 47.2			0
	ATOM	5788	N		A 369		7:494	-2.369	2.998	1.00 41.8	5		N
35	MOTA	5790	CA	ALA :	A 369	•	7.115	-3.346	1.966	1.00 38.5	6 · ·		С
	ATOM	5792	CB	ALA .	A 369		5.832	-2.891	1.277	1.00 40.4	0		С
	MOTA	5796	С	ALA .	A 369		8.162	-3.635	0.928	1.00 29.8	5		С
	MOTA	5797	Ο.	ALA .	A 369		9.095	-2.854	0.730	1.00 36.3	5		0
	MOTA	5 798	N	VAL .	A 370		7.966	-4.769	0.274	1.00 25.9	6		Ν.
40	ATOM	5800	CA	VAL .	A 370		8.831	-5.260	-0.769	1.00 29.5	7 .		С
	ATOM	5802	CB		A 370		9.849	-6.185	-0.229	1.00 26.2			Ċ
	ATOM	5804	CG1	VAL	A 370		10.757	-6.632	-1.321	1.00 32.4			С
	ATOM	5808	CG2	VAL	A 370		10.689	-5.482	0.827	1.00 30.9			С
	ATOM	5812	С	VAL	A 370		7.929	-5.941	-1.796	1.00 31.9			С
45	MOTA	5813	0	VAL	A 370			-6.866	-1.490	1.00 36.5			0
	MOTA	5814	N	GLU	A 371		7.945	-5.452	-3.029	1.00 33.2			N
	MOTA	5816.			A 371		6.979	-5.876	-3.989	1.00 28.6			С
	ATOM	5818	CB		A 371			-4.939		1.00 32.0			С
	ATOM	5821	CG			•	5.266	-4.723	-2.470	1.00 38.8			С
50	MOTA	5824	CD	GLU	A 371		4.374	-3.505 .		1.00 44.4			С
	MOTA	5825			A 371		3.119	-3.685	-2.230	1.00 55.9			0
	ATOM	5826	OE2	GLU	A 371		4.919		-2.177	1.00 45.3			0
	ATOM	5827	·C	GLU	A 371		7.625	-5.792	-5.338	1.00 34.4			С
	MOTA	5828	0	GLU	A 371		8.335	-4.857	-5.587	1.00 31.8			0
55	ATOM	5829	N	GLY	A 372		7.410	·-6.797	-6.201	1.00 41.4	5		N
	MOTA	5831	CA	GLY	A 372		7.862	-6.730	-7.585	1.00 44.3			C
	MOTA	5834	С	GLY	A 372		7.151	-7.793		1.00 49.6			C
	MOTA	5835	0	GLY	A 372		6.383	-8.580		1.00 48.5			0
	MOTA	5836	N	PRO	A 373		7.383	-7.862		1.00 50.5			N
60	MOTA	5837	CA	PRO	A 373		8.248		-10.495	1.00 49.6			С
	ATOM	5839	CB	PRO	A 373		8.726	-7.915	-11.588	1.00 51.1	.3		C

5	ATOM	5842	CG	PRO A 3	373		7.732	-9.025	-11.666	1.00	50.04				C ·
٦	ATOM	5845		PRO A		•			-10.531		50.00		• •		С
	ATOM	5848		PRO A			7.502		-11.212		51.84				С
•	ATOM	5849		PRO A			6.324		-11.428	1.00	59.43		•		0
		5850		PHE A			8.177		-11.584		53.98				N
10	MOTA	5852		PHE A			7.578		-12.360		55.44				С
10	MOTA			PHE A			7.709		-11.615	1.00	53.01				С
	MOTA	5854		PHE A			7.163	-2.396	-10.227	1.00	51.03				С
	MOTA	5857		PHE A			7.959		-9.179	1.00	47.22		•		C
	MOTA	5858		PHE A			7.448	-2.766	-7.895	1.00	52.78				С
1.0	MOTA	5860		PHE A			6.132	-2.437	-7.669	1.00	52.67				C
15	MOTA	5862		PHE A			5.326	-2.083			49.05				С
	MOTA	5864		PHE A			5.840	-2.063	-9.987		49.61			٠.	С
	MOTA	5866		PHE A			8.342		-13.656		57.87				С
	ATOM	5868	C	PHE A			9.536		-13.651		59.75				0
	MOTA	5869					7.692		-14.762		68.38	•			N
20	MOTA	5870	N	VAL A			8.440		-16.020		72.14				С
	MOTA	5872	CA	VAL A			7.752		-17.217		73.03				С
	MOTA	5874	CB	VAL A			8.601		-18.453		71.54				С
	MOTA	5876		VAL A			7.514		-16.966		72.18				С
	MOTA	5880		VAL A			0 757		-16.347		76.96				С
25	ATOM	5884	С	VAL A			7.909	-0 792	-16.840		79.60				0
	MOTA	5885	0	VAL A			10 008		-16.073		85.14				N
	ATOM	5886	N	THR A			10.529	0.219	-16.248		88.23	÷ .			С
	MOTA	5888	CA	THR A			11.255	0.210	-14.901		89.17	•			C.
	ATOM	5890	CB	THR A			11.233		-13.804		90.48	٠.			0
30	MOTA	5892		THR A			10.674	1 992	-14.352		86.17				С
	MOTA	5894		THR A			11.560	.0.063	-17.389		88.70				С
	MOTA	5898	· C	THR A			11.064	-1 086	-17.791		87.38				0
	MOTA	5899	0	THR A LEU A			12 114	1 155	-17.922		87.83				N
	MOTA	5900	N .	LEU A			13.111	0 969	-18.996		88.50				С
35	MOTA	5902	CA	LEU A			12.510	1 234	-20.409		90.35				C
	ATOM	5904	CB	LEU A			11.904		-21.438		89.96				С
	ATOM	5907	CG	LEU A			12.034		-22.783		89.80				С
	ATOM	5909		LEU A			12.520		-21.579		90.81				С
40	ATOM	5913		LEU A			14.475	1.712	-18.873		89.75				С
40	ATOM	5917	C O	LEU A			14.792		-17.889		82.52				0
	ATOM	5918	N.	ASP A			15.258		-19.937		92.45				N
	ATOM	5919		ASP A			16.640		-20.006		95.71				С
	MOTA	5921	CA CB	ASP A			17.018		7 -21.238		98.28				С
45	MOTA	5923 5926	CG	ASP A			17.513		-22.480		102.00				С
43	MOTA			ASP A			17.062	2.14:	3 -23.628		0101.56				0
	ATOM	5927 5928		ASP A		•	18.342		7 -22.402		0102.38				0
	MOTA	5920	C	ASP A			16.922		5 -18.610		94.33				С
	ATOM			ASP A			17.057		9 -18.295		96.66				0
٠.	ATOM	5930	0	MET A	379		16.945	1.35	9 -17.798		0 91.54			1	N ·
50	ATOM	5931	N C	MET A			17.353	1.32	8 -16.436		0 87.87				С
	MOTA	5933	CA	MET A			16.910		9 -15.863		0 83.99				C
	ATOM	5935	CB	MET A			15.410		2 -15.499		0 78.36				C
	ATOM	5938	CG	MET A			15.163		4 -14.259		0 66.38				S
	ATOM	5941	SD	MET A			15.285		6 -15.258		0 67.19			•	С
55	MOTA	5942		MET A			18.885		5 -16.353		0 89.93				C
	ATOM	5946		MET A			19.336		2 -15.998	1.0	0 89.20				. 0
	MOTA	5947		GLU A			19.666		2 -16.667		0 90.93				N
	MOTA	5948		GLU A	7 200		21.180		5 ~16.602		0 93.24				С
<i>c</i> o	MOTA	5950		GLU A	7 200		21.180		5 -17.575		0 92.65				С
60	MOTA	5952		GLU A	7 380		23.205		1 -17.244		0 91.21				С
	MOTA	לכצכ	CG	GTO E	, 200		20.200	1., 2.							

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5	ATOM	5958	CD	GLU A	.380	23.355	-1.819 -	15.836	1.00			С
J				GLU A		23.037	-3.027 -	15.615	1.00			0
	ATOM			GLU A		23.811	-1.058 -		1.00		•	0
	MOTA			GLU A		21.762	1.922 -	-16.785	1.00			С
	MOTA			GLU A		22.744	2.305 -	-16.108	1.00			0
10	MOTA			ASP A		21.142	2.717 -	-17.684	1.00	92.40		N
10	ATOM			ASP A		21.428	4.156 -		1.00			С
			СВ	ASP A		20.206	4.883 -		1.00	90.34		С
	ATOM		CG	ASP A		19.817	4.397 -	-19.774	1.00			·C .
	MOTA			ASP A		20.728	4.002 -	-20.536	1.001	01.01		0
15	MOTA			ASP A		18.627		-20.175	1.00	96.62		0
13	ATOM	•	C	ASP A		21.691		-16.531		83.94		С
	MOTA		Ö.	ASP A		22.594		-16.416		87.02		О
	ATOM	-	N ·	CYS A		20.883		-15.540		74.79		N
			CA	CYS A		20.891	5.209	-14.273	1.00	66.78		С
20	ATOM	-	CB	CYS P		19.874	4.543	-13.367	1.00	67.02		C
20	MOTA		SG	CYS A		18.314		-14.255	1.00	65.45		S
	MOTA		C	CYS A		22.273		-13.730	1.00	62.15		С
	MOTA	*	Ö	CYS F		22.585		-12.700	1.00	59.92		Ο.
	ATOM ATOM		N	GLY F		23.123		-14.447	1.00	61.83		Й
ລຣ໌		5987	CA		383	24.478		-14.011	1.00	66.26		C
25	MOTA	5990	C		383	25.143		-14.225		69.13		С
	MOTA	5991		GLY A		25.005	6.281	-15.266	1.00	70.50		0
	MOTA	5992	N .		A 384	25.854	6.144	-13.226	1.00	73.69		N
	MOTA	5994	CA		A 384	26.709		-13.454	1.00	77.96		С
30	ATOM	5996	CB		A 384	26.793		-12.245	1.00	81.61		С
30	MOTA	5999	CG		A 384	28.007		-12.283	1.00	85.12		С
	MOTA	6000		TYR		27.941	10.364			88.82		С
-	MOTA	6002	CE1		A 384	29.048	11.194	-12.893		87.19		С
	MOTA	6004	CZ		A 384	30.239	10.752	-12.358	1.00	90.20		C
35	ATOM	6005	OH		A 384	31.364		-12.375		89.10		0
33	ATOM ATOM	6007		TYR		30.320		-11.790		90.57		C
	ATOM	6009		TYR		29.208		-11.757	1.00	84.83		С
	ATOM	6011	C		A 384	28.056		-13.746		77.71		. С
	ATOM	6012	0		A 384	28.429		-13.131		75.56		0
40	ATOM	6013	N		A 385			-14.691		80.96		N
40	MOTA		CA		A 385			-15.125		82.76		С
	MOTA	6017	CB		A 385	4		-16.592		84.72		С
	MOTA	6020	CG		A 385			-16.736		87.65		С
	ATOM	6021			A 385			-16.404	1.00	85.93		0
45	ATOM	6022			A 385			-17.258	1.00	88.07	•	N
43	MOTA	6025	C		A 385		7.705	-14.990	1.00	83.09		C
	ATOM	6026	ō		A 385			-14.965		81.57		0
		6027			A 385			-14.908		82.17		0
	ATOM		N	SER				43.679		55.48		N
50	MOTA	6030	CA	SER				43.412	1.00	51.63		C.
50	ATOM	6032	СВ	SER				42.712	1.00	52.68		С
	ATOM	6035	OG	SER				42.380	1.00	49.83		0
. 1	ATOM	6037	c	SER				42.623	1.00	54.62		С
		6038	ō	SER				42.639	1.00	56.38		0
55	ATOM	6041	N	PHE				41.916	1.00	57.53		N
رر	ATOM	6043	CA	PHE						57.72		С
	MOTA MOTA	6045	CB	PHE					1.00	56.01		С
	ATOM	6048	CG	PHE						51.92		С
	ATOM	6049		1 PHE					1.00	50.49		C.
60	ATOM	6051		1 PHE					1.00	55.85		С
UU		6053	CZ	PHE					1.00	54.01		С
	ATOM	5033	-0	- 110	٠ بـ							

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27.077
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                                                         37.470
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5	MOTA	6168	С	LEU	В	6	11.446	68.653	37.996	1.00 4				С
	MOTA	6169	0 .	LEU	В	6	 11.394	68.726	39.205	1.00 5				0
	MOTA	6170	N	ARG	В	7	10.436	68.228	37.245	1.00 4				N
	ATOM	6172	CA	ARG	В	7	9.325	67.471	37.771	1.00 3				С
	ATOM	6174	CB	ARG	В	7	8.103	68.326	37.963	1.00 4				C
10	MOTA	6177	CG	ARG	В	7	8.306	69.383	39.081	1.00 4				C
	ATOM	6180	CD	ARG	В	7	7.066	70.215	39.470	1.00 4				C
	ATOM	6183	NE	ARG	В	7	6.508	70.882	38.289	1.00 6				N
	MOTA	6185	CZ	ARG	B.	7	5.417	71.659	38.262	1.00				С
	ATOM	6186	NH1	ARG	В	7	4.720	71.907	39.367	1.00				N
15	MOTA	6189	NH2	ARG	В.	7	5.021	72.192	37.118	1.00	66.22			N
	MOTA	6192	С	ARG	В	7	9.095	66.395	36.744	1.00 4				С
	ATOM	6193	0	ARG	В	7	9.743	66.393	35.697	1.00				0
	ATOM	6194	N	GLY	В	8	8.213	65.451	37.037	1.00				N
•	ATOM	6196	CA	GLY	В	8	7.775	64.510	36.017	1.00 4	44.58			С
20	ATOM	6199	Ċ	GLY	В	8	8.126	63.080	36.314	1.00 5				C
•	MOTA	6200	Ó	GLY	В	. 8	8.464	62.734	37.457	1.00				0
	ATOM	6201	N	LYS	В	9	8.059	62.251	35.270	1.00				N
	ATOM	6203	CA	LYS	В	9	8.331	60.829	35.404	1.00 !				С
	MOTA	6205	CB	LYS	В	9	7.136	60.163	36.102	1.00	63.35			C
25	ATOM	. 6208	CG	LYS	В	9	5.746	60.383	35.457	1.00				С
	MOTA	6211	ĊD	LYS	В	9	4.812	59.234	35.916	1.00				С
	MOTA	6214	CE	LYS	B	9	3.321	59.481	35.622	1.00				С
	ATOM	6217	NZ	LYS	B.	9	2.630	60.116	36.794	.1.00				N
	ATOM	6221	С	LYS		. 9	8.661	60.089	34.086	1.00				C
30	MOTA	6222	0	LYS	В	9 '	8.631	60.659	32.990	1.00				0
	ATOM	6223	N	SER	В	10	8.974	58.805	34.211	1.00			•	N
	MOTA	6225	CA	SER		10	9.357	57.968	33.073	1.00				С
	MOTA	6227	CB	SER		10	9.764	56.630	33.631	1.00				C
	ATOM	6230	OG	SER		10	 8.858	56.310	34.679					0
35	MOTA	6232	С	SER		10	8.256	57.723	32.029	1.00				C
	ATOM	6233	0	SER		10	8.509	57.692	30.820	1.00				0
	MOTA	6234	N	GLY		11	7.034	57.522	32.497	1.00				N C
	MOTA	6236	CA	GLY		11	5.913	57.328	31.607	1.00				c
40	MOTA	6239	C	GLY		11	5.615	58.594	30.850	$1.00 \\ 1.00$				0
40	ATOM	6240	0	GLY		11	5.172	58.582	29.710	1.00				N
	MOTA	6241	N	GLN		12	5.855	59.731 60.920	31.456 30.714	1.00				C
•	ATOM	6243	CA	GLN		12	5.495		31.404	1.00				c
	MOTA	6245	CB	GLN		12	4.324 3.241	61.552 60.485	31.587	1.00				c
45	ATOM	6248	CG	GLN GLN		12 12	1.931	61.070	31.972	1.00				c
43	ATOM	6251	CD OF 1	GLN		12	1.866	61.968	32.838	1.00				ő
•	ATOM	6252 6253		.GLN		12	0.862	60.578	31.346	1.00				N
	ATOM ATOM	6256				12	6.566	61.922	30.368					C
				GLN		12	6.322	62.740	29.514	1.00				ō
50	ATOM ·	6257	O '	GLY		13	7.747	61.848		1.00				Ŋ
50	ATOM	6258	N CA			13	8.778	62.837	30.689		52.72			C
•	ATOM	6260		GLY		13	9.039		31.852		51.10			Č
	ATOM		C	GLY		.13	8.229	63.885			47.37			ō
	MOTA	6264 6265	O N	GLY TYR		14	10.180	64.450			47.23			· N
55.	ATOM ATOM	6267	CA	TYR		14	10.685	65.341	32.818		48.86	•		C
JJ.				TYR			12.079	64.874	33.266		47.74		,	C
	MOTA	6269 6272	CB CG	TYR		14 14	12.061	63.570	34.037		45.03			č
	ATOM ATOM	6273		TYR		14	12.346	62.368	33.443		45.11			Č
	ATOM	6275		TYR		14	12.314	61.184			44.50			Ċ
60	ATOM	6277	CZ	TYR		14	11.978	61.258	35.556		45.22			C C
oo		6278	OH	TYR		14	11.908	60.155	36.388		45.51			ō
	MOTA	0210)II	111	נו	7.4	12.500	00.133	30.300	~				_

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1.00 37.21
                                                                                       С
                                       11.702 62.446
                                                       36.117
5
     MOTA
            6280
                  CE2 TYR B
                             14
                                                                                       C
                                       11.741
                                               63.566
                                                       35.378 1.00 43.77
            6282
                  CD2 TYR B
                              14
     MOTA
                                                                                       C
                                                                1.00 49.55
                                       10.776
                                               66.739
                                                        32.217
                              14
     MOTA
            6284
                  С
                       TYR B
                                                                                       0
                                                                1.00 52.45
                                       11.293
                                               66.888
                                                        31.111
                       TYR B
                              14
     ATOM
            6285
                  0
                                                                                     N
                                                        32.924
                                                                1.00 45.83
                                       10.286
                                               67.759
                              15
     ATOM
            6286
                  N
                       TYR B
                                                        32.339
                                                                                       C
                                                                1.00 39.66
                                               69.079
                                       10.233
                       TYR B
                              15
            6288
                  CA
10
     MOTA
                                                                1.00 39.42
                                                                                       C
                                               69.345
                                                        31.844
                       TYR B
                              15
                                        8.817
            6290
                  CB
     MOTA
                                                                                       C
                                        7.835
                                               69.394
                                                        32.978
                                                                1.00 40.57
            6293
                  CG
                       TYR B
                              15
     ATOM
                                                                                       С
                                                                1.00 43.59
                                        7.743
                                               70.510
                                                        33.798
                  CD1 TYR B
                              15
            6294
     ATOM
                                                                                       С
                                                                1.00 34.88
                  CE1 TYR B
                              15
                                        6.869
                                               70.561
                                                        34.824
     ATOM
            6296
                                                                                       C
                                                                 1.00 37.24
                                        6.065
                                                        35.062
                       TYR B
                                               69.496
            6298
                  CZ
                              15
15
     MOTA
                                                                                       0
                                                        36.110
                                                                 1.00 47.03
                       TYR B
                                        5.168
                                               69.511
                              15
     MOTA
            6299
                  OH
                                                                                       С
                                                        34.273
                                                                 1.00 41.16
                                               68.390
                              15
                                       6.130
            6301
                  CE2 TYR B
     ATOM
                                                                 1.00 42.00
                                                                                       С
                                               68.340
                                                        33.240
                  CD2 TYR B
                              15
                                       7.008
            6303
     MOTA
                                                                                       С
                                               70.194
                                                        33.276
                                                                 1.00 40.31
                                       10.686
     ATOM
            6305
                  С
                       TYR B
                              15
                                                                                       O
                                                        34.478
                                                                 1.00 37.96
                                       10.679
                                               70.062
                       TYR B
                              15
20
            6306
     MOTA
                  0
                                                                                       N
                                                                 1.00 43.44
                                       11.069
                                               71.312
                                                        32.676
                       VAL B
                              16
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            6307
                  N
                                                                                       C
                                                        33.369
                                                                 1.00 42.50
                                       11.673
                                               72.427
            6309
                       VAL B
                              16
     MOTA
                  CA
                                                        32.925
                                                                 1.00 40.97
                                               72.669
                                       13.141
                       VAL B
                              16
     MOTA
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                                                                 1.00 36.56
                                               73.090 31.465
                                       13.240
                   CG1 VAL B
                              16
            6313
     MOTA
                                                                                       С
                                                        33.699
                                                                 1.00 45.84
                                       13.724 - 73.752
                       VAL B
                              16
25
            6317
                   CG2
     MOTA
                                                                 1.00 46.17
                                                                                       С
                                       10.836
                                              73.605
                                                        32.964
                       VAL B
                              .16
            6321
                   С
     MOTA
                                                                                       0
                                                        31.818
                                                                 1.00 44.78
                              16
                                       10.405
                                               73.700
                       VAL B
            6322
                   0
     ATOM
                                                                                       N
                                                                 1.00 47.27
                       GLU B
                                       10.609
                                               74:497
                                                        33.910
                              17
     ATOM
            6323
                   N
                                                                                       С
                                                                 1.00 48.45
                                       9.788
                                               75.649
                                                        33.701
            6325
                   CA
                       GLU B
                              17
     ATOM
                                                        35.056
                                                                 1.00 50.22
                                                                                       С
                                               76.118
                                        9.314
                       GLU B
                               17
30
     MOTA
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                  ·CB
                                                        35.050
                                                                 1.00 49.63
                                        8.748
                                               77.518
                       GLU B
                               17
            6330
                   CG
     MOTA
                                               78.008
                                                        36.443
                                                                 1.00 52.98
                                                                                       C
                                        8.451
                       GLU B
                               17
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                                                                                       0
                                                        37.020
                                                                 1.00 56.17
                                       7.420
                                               77.598
                       GLU B
                               17
     MOTA
             6334
                   OE1
                                                                 1.00 62.26
                                                                                       0
                                       9.251
                                               78.812
                                                        36.957
                       GLU. B 1.17
                   OE2
     ATOM
             6335
                                                                 1.00 49.62
                                                                                       С
                                                        33.070
                       GLU B
                               17
                                       10.587
                                                76.771
35
             6336
                   С
     MOTA
                                                                 1.00 58.28
                                                                                        O
                                                        33.603
                                                77.156
                                       11.605
            6337
                   0
                       GLU B
                               17
     MOTA
                                                        31.949
                                                                 1.00 52.00
                                                                                       N
                                       10.130
                                               77.308
                       MET B
                               18
             6338
                   N
     MOTA
                                                                                        C
                                       10.821
                                                78.430
                                                        31.301
                                                                 1.00 52.60
             6340
                   CA
                       MET B
                               18
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                                                                 1.00 52.70
                                                                                        C
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                                                        29.976
             6342
                   CB
                       MET B
                               18
     MOTA
                                                                                        C
                                                                 1.00 55.57
                                       12.598
                                                77.016
                                                        30.128
                       MET B
                               18
40
             6345
                   CG
     MOTA
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                                                76.172
                                                        28.583
                       MET B
                               18
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                   SD
     ATOM
                                                        27.930
                                                                                        С
                                                                 1.00 52.14
                                       14.275
                                                77.236
             6349
                   CE
                       MET B
                               18
     ATOM
                                                         31.035
                                                                 1.00 50.66
                                                                                        C
                                        9.874
                                                79.625
                       MET B
     MOTA
             6353
                   С
                               18
                                                                 1.00 49.38
                                                                                        0
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                                                79.496
                                                         31.067
             6354
                       MET B
                               18
     ATOM
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                                                                                        N
                                       10.452
                                                80.786
                                                         30.780
                                                                 1.00 49.10
                       THR B
                               19
45
             6355
                   N
     MOTA.
                                                                                        С
                                                                 1,00 51.16
                                        9.650
                                                81.918
                                                         30.382
                       THR B
                               19
     MOTA
             6357
                   CA
                                                                                        С
                                                         31.355
                                                                 1.00 50.92
                                        9.716
                                               83.092
             6359
                       THR B
                               19
                   CB
     MOTA
                                                                                        0
                                                                1.00 46.48
                                                         31.217
                                       10.956
                                                83.832
                   OG1 THR B
                               19
     ATOM
             6361
                                                         32.767 1.00 52.58
                                                                                        C
                                                82.591
                                       9.658
             6363
                   CG2 THR B
                               19
     MOTA
                                                82.426
                                                         29.041
                                                                 1.00 55.56
                                                                                        C
                                        10.084
                       THR B
                               19
50
     MOTA
             6367
                   С
                                                                                        0
                                        11.269 82.597
                                                         28:768
                                                                 1.00 55.44
             6368
                       THR B
                               19
                   0
     MOTA
                                        9.090
                                                82.685
                                                         28.214
                                                                 1.00 57.24
                       VAL B
             6369
                   N
                               20
     MOTA
                                                                                        C
                                                83.161
                                                         26.880
                                                                 1.00 54.55
                       VAL B
                                        9.307
             6371
                   CA
                               20
     ATOM
                                                                                        C
                                                82.067
                                                         25.827
                                                                 1.00 54.27
                                         8.940
                   CB
                       VAL B
                               20
     ATOM.
             6373
                                                                                        Ċ
                                         9.851
                                                80.829
                                                         25.982
                                                                 1.00 54.44
                   CG1 VAL B
55
             6375
                               20 .
     ATOM
                                                                                        С
                                                         25.953
                                                                 1.00 55.00
                   CG2 VAL B
                               20
                                         7.504
                                                81.630
             6379
      MOTA
                                                                                        C
                                                         26.771
                                                                 1.00 55.62
                                                84.325
                                         8.377
             6383
                   С
                        VAL B
                               20
      ATOM
                                                84.209
                                                         27.224
                                                                 1.00 55.85
                                         7.234
                        VAL B
                               20
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      ATOM
                                         8.875
                                                85.444
                                                         26.223
                                                                 1.00 56.40
             6385
                   N
                        GLY B
                               21
      MOTA
                                                                                        С
                                                         25.916
                                         8.066
                                                86.620
                                                                 1.00 54.12
 60
             6387
                   CA
                        GLY B
                               21
     ATOM
                                         8.292 .87.912
                                                         26.694
                                                                  1.00 52.80
             6390
                   C
                        GLY B
                               21
      MOTA
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										•			
5	ATOM	6391	o ·	GLY :	B 23		8.913	87.910	27.737	1.00 45.49	•		0
	ATOM	6392	N	SER			7.772	89.020	26.147	1.00 52.10			N
	ATOM	6394	CA	SER			7.729	90.308	26.811	1.00 45.9			
	ATOM	6396	CB	SER			8.740	91.218					C
									26.200	1.00 48.74			, C
10	MOTA	6399	OG	SER			10.028	90.606	26.262	1.00 58.03			0
10	MOTA	6401	С	SER			6.328	90.918	26.679	1.00 51.6			С
	ATOM	6402	0	SER			5.916	91.373	25.610	1.00 48.63	3		0
	ATOM	6403	N	PRO 1	B 23		5.587	90.895	27.784	1.00 51.99	j .		N
	ATOM	6404	. CA	PRO 1	B 23		6.088	90.276	29.019	1.00 51.30) .		С
	ATOM	6406	CB	PRO I	B 23		4.902	90.437	29.964	1.00 54.52			C
15	ATOM	6409	CG	PRO I			3.759	90.424	29.043	1.00 50.00			Ċ
	ATOM	6412	CD	PRO			4.226	91.436	27.979	1.00 49.63			Ċ
	ATOM	6415	C	PRO			6.368			1.00 47.00			
	ATOM			PRO I				88.800	28.881				C
		6416	0				5.860	88.229	27.944	1.00 48.90			0
00	ATOM	6417	N	PRO I			7.169	88.249	29.794	1.00 53.61			N
20	MOTA	6418	CA	PRO 1			7.415	86.787	30.020	1.00 54.15	5		С
	ATOM	6420	CB	PRO 1	B 24		8.155	86.804	31.345	1.00 51.32	2		С
	ATOM	6423	CG	PRO I	B 24		8.902	88.094	31.318	1.00 50.72	?		С
	ATOM	6426	CD	PRO 1	B 24		7.995	89.088	30.680	1.00 53.02	2		С
	ATOM	6429	С	PRO I	B 24		6.260	85.781	30.261	1.00 55.63			C
25	ATOM	6430	0	PRO 1			5.567	85.900	31.270	1.00 54.27			ō.
	ATOM	6431	N	GLN I			6.097	84.775	29.392	1.00 57.58			N
	ATOM	6433	CA	GLN I			5.025	83.775	29.524	1.00 56.58			
		6435	CB	GLN I									. C
	ATOM						4.404	83.453	28.153	1.00 58.02			. С
20	ATOM	6438	.CG	GLN I			3.196	84.297	27.785	1.00 61.39			С
30	ATOM	6441	CD	GLN I			2.729	84.086	26.353	1.00 63.09			С
•	ATOM	6442		GLN I			2.293	82.981	25.990	1.00 69.50)		0
	ATOM	6443	NE2	GLN I	B 25		2.802	85.135	25.543	1.00 54.53	L		N
	ATOM	6446	. C	GLN I	B 25	•	5.604	82.496	30.116	1.00 58.86	• •		С
	ATOM	6447	0	GLN I	B 25		6.574	81.987	29.559	1.00 57.53	3	•	0
35 ·	ATOM	6448	N	THR I			5.036	82.000	31.228	1.00 52.25			N
	ATOM	6450	CA	THR I			5.497	80.785	31.866	1.00 49.89			c
	ATOM	6452	CB	THR I			5.043	80.761	33.304	1.00 51.53			C
. '	ATOM	6454		THR I			5.882	81.592	34.127				
	ATOM	6456		THR I			5.233			1.00 48.51			0
40	ATOM	6460	C					79.353	33.886	1.00 49.37			C
70				THR I			4.970	79.505	31.224	1.00 51.74			, C
	MOTA	6461	0	THR I			3.772	79.321	31.123	1.00 55.36			0
	MOTA	6462	N	LEU I		•	5.861	78.603	30.808	1.00 52.47			N
	ATOM	6464	CA	LEU I			5.440	77.291	30.296	1.00 52.98	}		С
	ATOM	6466	CB	LEU I	B 27		5.447	77.292	28.768	1.00 53.80)		С
45	MOTA	6469	CG	LEU I	B 27		4.766	78.485	28.088	1.00 55.67	1		С
	MOTA	6471	CD1	LEU I	B 27		5.163	78.522	26.640	1.00 52.93			С
	MOTA	6475	CD2	LEU I	В 27		3.248	78.447	28.216	1.00 52.46			C
	ATOM	6479		LEU I			6.344	76.152		1.00 54.38			č
	ATOM	6480	ō	LEU I			7.492	76.415	31.190				
50	ATOM	6481		ASN I			5.809			1.00 55.85			0
50								74.922	30.863	1.00 51.66			· N
	MOTA	6483	CA	ASN I			6.518	73.711	31.292	1.00 55.85			С
	ATOM	6485	CB.	ASN I			5.526		31.940	1.00 58.80			С
	MOTA	6488	CG	ASN I			5.260	72.950	33.449	1.00 57.89)		С
	MOTA	6489	OD1	ASN I	B 28		4.145	72.685	33.961	1.00 43.49)		0
55	ATOM	6490	ND2	ASN I	B 28		6.273	73.440	34.152	1.00 52.67	,		N
	MOTA	6493	С	ASN I			7.119	73.035	30.037	1.00 54.00			C.
	ATOM	6494	0	ASN I			6.411	72.858	29.040	1.00 55.20			ŏ
	ATOM	6495	N	ILE I			8.385	72.602	30.082	1.00 33.20			N
	ATOM	6497	CA	ILE I			9.090	72.101					
60		6499	CB	ILE E						1.00 41.75			C
w	ATOM						10.096	73.201	28.430	1.00 41.61			. C
	MOTA	6501	CGI	ILE I	В 29		9.403	74.521	28.502	1.00 36.87	,		С

5	ATOM	6504	CD1	ILE E	a 2	29	8.620	74.882	27.272	1.00 35.29			С
J	ATOM	6508		ILE I		29	10.627	72.989	27.001	1.00 45.92			С
	ATOM	6512		ILE I		29	9.834	70.738	29.020	1.00 41.21			С
	MOTA	6513		ILE I		29	10.821	70.657	29.735	1.00 40.42			0
	MOTA	6514		LEU I		30	9.363	69.67.9	28.344	1.00 40.94			N
10	MOTA	6516		LEU I		30	10.056	68.371	28.308	1.00 42.00			С
10		6518		LEU I		30	9.450	67.507	27.215	1.00 41.64			С
	ATOM	6521		LEU		30	9.943	66.065	27050	1.00 41.51			Ç
	MOTA			LEU I		30	8.966	65.054	27.427	1.00 38.45			С
	MOTA	6523		LEU I		30 ·	10.258	65.805	25.617	1.00 51.30		•	С
15	ATOM	6527		LEU I		30	11.529	68.607	27.974	1.00 46.49			С
15	MOTA	6531		LEU I		30	11.849	69.519	27.220	1.00 47.11			0
	ATOM	6532		VAL 1		31	12.414	67.781	28.527	1.00 46.41			N
	ATOM	6533		VAL		31	13.858	67.880	28.288	1.00 47.73			С
•	ATOM	6535		VAL		31	14.633	67.834	29.620	1.00 48.19			С
20	MOTA	6537		VAL :		31	16.047	67.314	29.431	1.00 52.74			С
20	ATOM .	6539		VAL		31	14.661	69.187	30.226	1.00 47.82			С
	ATOM	6543		VAL.		31	14.251	66.709	27.422	1.00 49.66			С
	MOTA	6547	C	VAL		31	14.369	65.614	27.935	1.00 50.43			0
	MOTA	6548	0	ASP		32	14.488	66.937	26.122	1.00 50.95			N
25	ATOM	6549		ASP		32 ·	14.599	65.825	25.165	1.00 50.66			С
25	MOTA	6551		ASP		32	13.547		24.085	1.00 46.26			· C
	ATOM	6553	CB CG	ASP		32 32	13.417	64.802	23.209	1.00 46.83			С
	ATOM.	6556		ASP		32	12.601	63.952	23.614	1.00 57.65	•		0
	ATOM	6557		ASP		32 32	14.037	64.597	22.118	1.00 28.18			0
.20	ATOM	6558		ASP		32 32	15.937	65.627	24.483	1.00 50.93			C
30	MOTA	6559	C O	ASP		32	16.137	66.095	23.372	1.00 56.78			Ō
	ATOM	6560	N	THR		33	16.854	64.901		1.00 44.66			N
	MOTA	6561	CA	THR		33	18.135	64.814	24.467	1.00 41.11			С
	ATOM	6563	CB	THR		33	19.151	64.207	25.419	1.00 44.39			С
35	MOTA	6565 6567		THR		33	18.649	62.989	25.966	1.00 47.50			Ò
33	ATOM .	6569		THR		33	19.298	65.077	26.643	1.00 45.76			С
	ATOM	6573	C	THR		33 .	18.075	64.056	23.159	1.00 43.39			С
	ATOM	6574	Ö	THR		33	19.101	63.882	22.521	1.00 45.31			0
•	ATOM	6575	ท	GLY		34	16.891	63.610	22.749	1.00 43.77			N
40	ATOM	6577	CA	GLY		34	16.739	62.822	21.528	1.00 46.99			С
40	ATOM	6580	C	GLY		34	16.380	63.629	20.282	1.00 49.16			С
	ATOM	6581	Ö	GLY		34	16.324	63.093	19.151	1.00 50.21			0
	ATOM	6582	N	SER		35	16.151	64.924		1.00 50.26			N
	ATOM	6584	CA	SER		35	15.776	65.838	19.394	1.00 47.28			С
45	ATOM	6586	СВ	SER		35	14.281	66.025	19.398	1.00 43.53			. C
43	ATOM	6589	OG	SER		35	13.916	66.661	20.582	1.00 41.18	•		Q
	ATOM	6591	C.	SER.		35	16.491	67.207	19.504	1.00 43.05			С
-	ATOM	6592	ō	SER		35	17.273	67.446	20.440	1.00 43.12			0
	ATOM	6593	N	SER		36	16.238	68.094	18.549	1.00 37.14			. N
50	ATOM .	6595	CA	SER		36	16:982	69.332	18.512	1.00 36.80			С
50	ATOM	6597	CB	SER		36	18.137			1.00 40.35			C
	ATOM	6600	OG	SER		36	19.229	68.365	18.021	1.00 36.18			0
	MOTA	6602	C	SER		36	16.182	70.629	18.297	1.00 42.36			С
	ATOM	6603	ō	SER		36	16.739	71.718	18.339	1.00 49.70		•	. 0
55	ATOM	6604	N	ASN		37	14.879	70.560	18.107	1.00 45.23			N
,,,	ATOM	6606	· CA	ASN-			14.135	71.783	17.906	1.00 44.85			С
•	ATOM	6608	CB	ASN		37	13.080	71.617	16.845	1.00 43.43		٠.	С
	ATOM	6611	CG	ASN		37	13.659	71.592	15.492	1.00 49.01			С
	ATOM	6612		ASN		37	14.303			1.00 53.37			0
60	ATOM	6613		ASN		37	13.450		14.715	1.00 47.23			N.
00	ATOM	6616	C	ASN		37	13.432		19.164	1.00 43.89			C
	¥10M	0010	C	いいれ		J.							•

5	ATOM	6617	0	ASN B	37		12.955	71.279	19.843	1.00 48.92			0
	ATOM	6618	N	PHE B.	38.	٠,	13.379	73.447	19.454	1.00 39.62			N
	ATOM	6620		PHE B	38		12.666	73.984	20.588	1.00 37.09			С
•	ATOM	6622	СВ	PHE B	38		13.518	75.084	21.189	1.00 34.12			С
	ATOM	6625	CG	PHE B	38		12.915	75.809	22.291	1.00 36.88			С
10	ATOM	6626	CD1	PHE B	38		13.190	77.128	22.451	1.00 43.04			С
	ATOM	6628		PHE B	38		12.639	77.847	23.480	1.00 43.52			С
	ATOM	6630	CZ	PHE B	38		11.810	77.261	24.366	1.00 45.02			С
	ATOM	6632		PHE B	38		11.519	75.950	24.235	1.00 51.64			С
	ATOM	6634		PHE B	38		12.082	75.213	23.185	1.00 52.30			С
15	ATOM	6636	C	PHE B	38		11.313	74.445	20.010	1.00 40.81	•		С
13	ATOM	6637	ō	PHE B	38		11.241	75.206	19.018	1.00 42.46			0
	ATOM	6638	N	ALA B	39		10.238	73.940	20.607	1.00 40.42			N
	MOTA	6640	CA	ALA B	39		8.903	74.198	20.105	1.00 44.90			С
• .	ATOM	6642	CB	ALA B	39		8.473	73.061	19.113	1.00 45.36			C
20	ATOM	6646	C	ALA B	39		7.889	74.308	21.212	1.00 41.28			С
20	ATOM	6647.	o	ALA B	39		7.961	73.617	22.213	1.00 44.60		-	0
	ATOM	6648	N	VAL B	40		6.929	75.177	21.046	1.00 40.49	_		N
		6650	CA	VAL B	40		5.885	75.186	22.027	1.00 49.83			С
	MOTA		CB	VAL B	40		6.020	76.354	22.997	1.00 49.55			С
25	ATOM	6652		VAL B	40		7.345	76.332	23.631	1.00 46.17			С
.25	MOTA	6654			40		5.830	77.657	22.280	1.00 54.69			С
	MOTA	6658		VAL B			4.496	75.202	21.404	1.00 51.60			Ċ
	MOTA	6662	C	VAL B	40		4.209	75.202	20.435	1.00 56.20			ō
	ATOM	6663	0	VAL B	40		3.629	74.394	21.958	1.00 50.81			N
20	ATOM	6664	N	GLY B	41		2.235	74.528	21.608	1.00 54.35			C
30	ATOM	6666	CA.	GLY B	41	·		76.000	21.658	1.00 54.27			Ċ
	MOTA	6669	C	GLY B	41		1.861		22.646	1.00 50.40			ō
	ATOM	6670	0	GLY B	41		2.139	76.439	20.585	1.00 55.45		٠.	N
	MOTA	6671		ALA B	42		1.208	77.840	20.303	1.00 57.72			C
25	ATOM	.6673	CA	ALA B	42		0.864	78.375	19.208	1.00 57.72			č
35	ATOM	6675	CB	ALA B	42				20.158	1.00 59.93			č
	MOTA	6679	C	ALA B	42		-0.620	78.089	19.956	1.00 54.51			ő
	ATOM	6680	0	ALA B	42		-1.041		20.205	1.00 59.25			N
	MOTA	6681	N	ALA B	43		-1.422	77.028	19.904	1.00 58.08	•		c
40	MOTA	6683	CA	ALA B	43		-2.838	77.148	18.403	1.00 57.09			č
40	ATOM	6685	CB	ALA B	43		-3.069	76.951	20.669	1.00 57.05			č
	MOTA	6689	C	ALA B	43		-3.577	76.084	20.869	1.00 57.71			ŏ
	MOTA	6690	0	ALA B	43		-3.047	75.011	21.067	1.00 58.13			Ŋ
	ATOM	6691	N	PRO B	44		-4.809	76.358	21.856	1.00 55.97			C
4.5	MOTA	6692	CA	PRO B	44		-5.568	75.407	21.550	1.00 57.92			Ċ
45	ATOM	6694	CB	PRO B	44		-7.009	75.819	20.407	1.00 57.30			č
	ATOM	6697	CG	PRO B	44		-6.845	76.827					C
	MOTA	6700	CD	PRO B			-5.628	77.554	20.804	1.00 57:17			c
	ATOM	6703	С	PRO B			-5.339		21.388	1.00 55.26			O.
	ATOM	6704	, О	PRO B			-5.058	73.798	20.199	1.00 55.54			
50	ATOM .		N	HIS B			-5.458	73.083					N C
	ATOM	6707	CA	HIS B			-5.380	71.662	22.074				
	ATOM	670,9	CB	HIS B	45		-3.960			1.00 47.73	••		C
	ATOM	6712	CG	HIS B	45		-3.854	69.743	21.624	1.00 47.10			C
	ATOM	6713	ND1	HIS B	45		-3.661		22.613	1.00 47.83			N
55	MOTA	6715	CE1	HIS B	45		-3,628		22.062				С
	MOTA	6717		HIS B			-3.798		20.755	1.00 39.59			N
	ATOM	6719		HIS B			-3.932			1.00 37.38			C
	ATOM	6721	С	HIS B			-5.990	71.052					С
	ATOM	6722	0	HIS B	45		-5.850	71.599					0
60	ATOM	6723	N	PRO B			-6.670	69.930					N
	ATOM	6724	CA	PRO E			-7.391		24.372	1.00 58.25			С
				-									

5	3 TOM	6726	СВ	PRO B	46		-8.093	68.157	23.840	1.00 5				С
3	MOTA		-	PRO B			-8.000	68.181	22.353	1.00 5				C.
•	MOTA	6729		PRO B	46		-6.815	69.046	22.032	1.00 6				С
	ATOM	6732	-	PRO B	46		-6.491	69.075	25.575	1.00 5	57.99			С
	ATOM	6735	-		46	•	-6.953	68.992	26.716	1.00 5			•	0
	MOTA	673.6		PRO B			-5.206	68.871	25.356	1.00 5				N
10	ATOM	6737	N	PHE B			-4.396	68.376	26.470	1.00 5				С
•	MOTA	6739	CA	PHE B				67.274	25.982	1.00 4				С
	ATOM .		CB	PHE B	47		-3.499	66.044	25.604	1.00 4				С
	MOTA	6744	CG	PHE B			-4.234	65.093	24.782	1.00 4				С
	MOTA	6745		PHE B			-3.640		24.702	1.00				C
15	MOTA	6747		PHE B			-4.315	63.949	24.429	1.00				Ċ
	MOTA	6749	CZ	PHE B			-5.596	63.746		1.00				Ċ.
	MOTA	6751		PHE B			-6.205		25.729	1.00				č
	ATOM	6753	CD2	PHE B			-5.530	65.822	26.070					Č
•	MOTA	6755	С	PHE B			-3.532	69.385	27.152	1.00				Ċ
20	ATOM	6756	0	PHE B	47		-2.763	69.015	28.046	1.00				N
	ATOM	6757	N .	LEU B	48		-3.661	70.647	26.760	1.00				
	ATOM	6759	CA	LEU B	48		-2.719	71.620	27.207	1.00				C.
	ATOM	6761	CB	LEU B	48		2.107	72.333	26.014	1.00				C
	ATOM	6764	CG	LEU B	48		-1.214	71.667	24.990	1.00				C
25	ATOM	6766		LEU B	48		-1.252	72.578	23.755	1.00				C
23	MOTA	6770		LEU B			0.179	71.567	25.528	1.00				С
•	ATOM	6774	C	LEU B			-3.453	72.636	27.955	1.00				С
	ATOM	6775	ō	LEU B			-4.383	73.194	27.396	1.00				0
	ATOM	6776	N	HIS E			-3.033	72.940	29.181		57.93		•	N
30		6778	CA	HIS E			-3.757	73.897	30.015		56.76	•		С
30	MOTA	6780	CB	HIS E			-3.451	73.706	31.497	1.00	61.80			C
	ATOM	6783	CG	HIS E			-4.070	72.466	32.048	1.00	67.51			C
	ATOM			HIS E			-5.274	71.984	31.583	1.00	65.77			N.
	ATOM	6784		HIS E			-5.579		32.226		68.88			С
	MOTA	6786					-4.615	70.615	33.092		72.14			N
35 .	MOTA	6788		HISE			-3.654	71.596	32.999		70.39			C
	MOTA	6790		HIS F			-3.484	75.276	29.617		55.32			Ċ
	ATOM	6792	C.	HIS H			-4.365	76.100	29.747		54.19		•	0
	ATOM	6793	0	HIS H			-2.278	75.563	29.139		57.08			N
	MOTA	6794	N	ARG I			-1.920	76.933	28.702		52.78			С
40	MOTA	6796	CA	ARG I				77.660	29.796		48.76			, C
	MOTA	6798	CB	ARG I			-1.133		30.591		53.36			C
	MOTA	6801	CG	ARG I			-0.218	76.713			54.71			Ċ
	MOTA	6804	CD	ARG I			0.743	77.384	31.593		61.19			N
	MOTA	6807	NE	ARG T			1.853	76.474	31.868		59.08		•	c
45	MOTA	6809	CZ	ARG			2.737							Ň
•	ATOM	6810		. ARG			2.693	1.			60.26			N
,	ATOM	6813	NH2	ARG	B 50		3.681				66.01			C
	MOTA	6816	С	ARG .	в 50		-1.078	76,790			54.68			_
	MOTA	6817	0	ARG	в 50		-0.699			1.00	57.99			0
50	MOTA	6818	N	TYR	B 51			77.896			55.14			N
	ATOM	6820	CA	TYR			0.040	77.836			51.39			C.
•	MOM	6822	СВ	TYR			-0.692	77.265	24.296		52.11			C.
	ATOM	6825		TYR			-1.939	77.986	23.819		50.59			,C
	ATOM	6826		TYR			-1.872				53.23			C
55	ATOM	6828		TYR:			-3.007				54.06			С
رر		6830					-4.238				56.68			· C
	ATOM						-5.428				55.76		•	0
	MOTA	6831		2 TYR			-4.311				56.57			С
	ATOM	6833		2 TYR			-3.178				55.59			С
20	ATOM	6835					0.654				49.19			С
60	ATOM	6837		TYR			0.394		25.825		48.94			0
	MOTA	6838	0	TYR	יור פ		0.335							

. 5	ATOM	6839	N	TYR	В	52	1.503	79.151	24.193	1.00 47.59		N
	ATOM	6841	CA	TYR	В.	52	2.182	80.378	23.852	1.00 50.52		С
	ATOM	6843	CB	TYR	В	52	3.496	80.019	23.199	1.00 44.85		С
	MOTA	6846	CG	TYR	В	52	4.382	81.161	22.853	1.00 43.08		С
	ATOM	6847	CD1	TYR	В	52	4.498	82.273	23.656	1.00 45.53		С
10	MOTA	6849	CE1	TYR	В	52	5.355	83.314	23.297	1.00 43.96		С
	ATOM	6851	CZ	TYR	В	52	6.080	83.202	22.134	1.00 41.86		С
	ATOM	6852	ОН	TYR	В	52	6.952	84.165	21.695	1.00 54.44		0
	ATOM	6854	CE2	TYR	·B	52	5.969	82.123	21.357	1.00 43.09	•	C
	ATOM	6856		TYR		52	5.138	81.113	21.705	1.00 46.61		С
15	ATOM	6858	С	TYR		52	1.327	81.241	22.914	1.00 53.39		С
	ATOM	6859	o	TYR	В	52	0.897	80.763	21.840	1.00 55.11		0
	ATOM	6860	N	GLN		53	1.066	82.488	23.312	1.00 49.66		N
	MOTA	6862	CA	GLN		53	0.350	83.402	22.424	1.00 53.39		С
•	ATOM	6864	СВ	GLN		53	-0.928	83.978	23.029	1.00 57.67		С
20	ATOM	6867	CG	GLN		53	-1.673	83.154		1.00 58.49		. C
	ATOM	6870	CD	GLN		53	-2.674	84.056	24.766	1.00 63.66		С
	ATOM	6871		GLN		53	-2.341	84.707	25.784	1.00 62.18		0
	ATOM	6872		GLN		53	-3.891	84.146	24.200	1.00 60.51		N
	ATOM	6875	С	GLN		53	1.254	84.569	21.988	1.00 54.38		С
25	ATOM	6876	ō	GLN		53	1.569	85.510	22.750	1.00 49.25	٠	ō
25	ATOM	6877	N	ARG		54	1.657	84.494	20.735	1.00 50.22		. N
	ATOM ·	6879	CA	ARG		54	2.547	85.458	20.202	1.00 45.95		C
•	ATOM	6881	СВ	ARG		54	2.907	85.045	18.778	1.00 45.10		Ċ
	ATOM	6884	CG	ARG		54	3.655	83.672	18.783	1.00 39.53		Ċ
30	ATOM	6887	CD	ARG		54	3.679	82.890	17.474	1.00 42.75		Č
30	ATOM	6890	NE	ARG		54	2.387	82.353	17.079	1.00 47.37		N
	ATOM	6892	CZ	ARG		54	2.139	81.788	15.910	1.00 45.51		c
	ATOM	6893		ARG		54	3.100	81.680	15.024			N
	ATOM	6896		ARG		54	0.931	81.330	15.618	1.00 42.27		N
35	ATOM	6899	С	ARG		54	1.939	86.836	20.386	1.00 52.82		c
33	ATOM	6900	ō	ARG		54	2.439	87.560	21.225	1.00 59.82		Ö
	ATOM	6901	N	GLN		55	0.855	87.196	19.686	1.00 57.85		N
•	ATOM	6903	CA	GLN		55	0.303	88.572	19.736	1.00 57.16		C
	MOTA	6905	CB.	GLN		55	-1.194	88.640	19.347	1.00 62.44		Ċ
40	ATOM	6908	CG	GLN		55	-1.469	88.563	17.810	1.00 70.53		č
	ATOM	6911	CD	GLN		55	-2.978	88.687	17.382	1.00 79.43		Ċ
	ATOM	6912		GLN		55	-3.369	89.660	16.701	1.00 80.66		Ō
	ATOM	6913		GLN		55	-3.802	87.692	17.764	1.00 79.42		N
	ATOM	6916	C	GLN		55	0.533	89.312	21.058	1.00 57.92		Ċ
45	ATOM	6917	ō	GLN		55	0.360		21.117	1.00 56.14	-	ō
•••	ATOM		N	LEU		56	0.930	88.622	22.121	1.00 55.89		Ŋ
	ATOM	6920	CA	LEU			1.213	89.336	23.370	1.00 58.18		C
	ATOM	6922	CB	LEU		56	0.712	88.524		1		
	ATOM	6925	CG	LEU			-0.721	88.029	24.402	1.00 62.37		C C
50	ATOM.	6927		LEU		-56	-1.296	87.699	25.797	1.00 63.41		č
50	ATOM	6931				56	-1.598	89.054	23.676	1.00 62.35		c
		6935	C	LEU		56	2.666	89.723		1.00 60.41		c
	ATOM ATOM	6936	ŏ	LEU		56	2.861	90.367	24.719	1.00 60.04	•	0.
		6937	- N	SER		57	3.663	89.348	22.857	1.00 57.76		N
55	MOTA		CA									C
33	ATOM	6939 6941	CB	SER		57 57	5.071	89.701	23.116	1.00 54.64		C
	ATOM	6941 6944		SER		57	5.991	88.475	23:117	1.00 56.81		
	MOTA		OG C	SER		57	7.344 5.661		23.423	1.00 54.08		0 C
	MOTA	6946	C	SER		57	5.658	90.710	22.153	1.00 53.95		
60	MOTA	6947	O M	SER		57		90.533		1.00 55.46		0
60	ATOM	6948	N	SER		58	6.218	91.755	22.738	1.00 52.39		N
	MOTA	6950	CA	SER	В	58	6.758	92.873	22.011	1.00 46.14		С

5	ATOM	6952	CB	SER I	3	58 .		6.820	94.070	22.947		47.29			C
	ATOM	6955	OG	SER I	3	58 ~		7.567	93.825	24.116		47.06	• :	:	0
	ATOM	6957	С	SER I	3	58		8.114	92.536	21.420		47.84			C.
	MOTA	6958	0	SER I	3	58		8.576	93.177	20.478		47.48			0
	ATOM	6959	N	THR 1	3	59		8.747	91.510	21.965		48.33			N
10	MOTA	6961	CA	THR I	3	59		10.006	91.008	21.429		42.92			C
	ATOM	6963	CB	THR I	3	59		10.885	90.549	22.559		42.65			C
	ATOM	6965	OG1	THR I	В	59		10.128	89.795	23.523		49.24			0
	ATOM	6967	CG2	THR I	B	59		11.359	91.709	23.347		45.57			C
	ATOM	6971	C	THR I	В	59		9.812	89.853	20.405		45.53			C
15	MOTA	6972	0	THR 1	В	59		10.800	89.319	19.883		42.19			0
	ATOM	6973	N	TYR I	В	60		8.566	89.465	20.113		44.25	٠.		N
	MOTA	6975	CA	TYR I	В	60		8.312	88.440	19.089		42.52			C
	MOTA	6977	CB	TYR I	В	60		6.854	88.060	19.079		42.61			C
٠.	ATOM	6980	CG	TYR :	В	60	•	6.444	87.188	17.912		39.56			C
20	ATOM	6981	CD1	TYR :	В	60		6.853	85.902 _.	17.825		39.91			C·
	MOTA .	6983	CE1	TYR	В	60		6.478	85.088	16.766		37.80			C
	ATOM	6985	CZ	TYR	В	60		5.693	85.576	15.787		41.24			С
•	ATOM	6986	OH	TYR	В	60		5.341	84.743	14.726		49.70			0
	ATOM	6988	CE2	TYR	В	60		5.263	86.875	15.855		38.20			C
25	MOTA	6990	CD2	TYR	В	60 ·		5:636	87.661	16.909		40.65			C
	ATOM	6992	C	TYR	В	60		8.593	88.944	17.691		47.70		•	C
	ATOM	6993	0	TYR	В	60		8.100	89.986	17.310		45.23			0
	ATOM	6994	N	ARG	В	61		9.376	88.195	16.913		53.11		·	N
	ATOM	6996	CA	ARG	В	61	•	9.536	88.482	15.488		47.96			C
30	ATOM	6998	CB	ARG	В	61		10.866	89.084	15.173		48.51			C
	ATOM	7001	CG	ARG	В	61		11.328	90.014	16.186		47.51			C
	ATOM	7004	CD	ARG	В	61		12.777	90.163	16.129		46.49			C
	MOTA	7007	NE	ARG	В	61 .		13.175	91.480	16.568		53.97			N
	ATOM	7009	CZ	ARG	В	61		14.425	91.808	16.746		57.00			C
: 35	ATOM	7010	NH1	ARG	В	61	•	15.338	90.893	16.529		62.31			N
	MOTA	7013	NH2	ARG	В	61		14.778	93.015	17.141		55.13			N
	ATOM	7016	С	ARG	В	61		9.346	87.181	14.730		48.27			C
	MOTA	7017	0	ARG		61		9.609	86.115	15.238		52.99			0
	MOTA	7018	N	ASP	В	62		8.910	87.304	13.496		44.77			N
40	ATOM	7020	CA	ASP	В	62		8.336	86.217	12.776		46.62			C
	MOTA	7022	CB	ASP	В	62		6.934	86.722	12.384		49.17			C C
	MOTA	7025	CG	ASP		62		6.177	85.815	11.468		53.87			
	MOTA	7026	OD1	ASP	В	62		6.754	84.805	11.004		55.89			0
	MOTA	7027	OD2	ASP		62		4.965	86.076	11.152		54.79			C
45	MOTA	7028	С	ASP		62		9.225	85.892	11.608		49.58			0
	MOTA	7029	0	ASP.		62		9.620	86.763	10.849		55.62			
	MOTA	7030	N	LEO		63		9.559	84.624	11.453		45.53			N C
	MOTA	7032	CA	LEU		63		10.464	84.255	10.394		42.20			
	ATOM	7034	CB	LEU		63		11.360	83.083	10.835		41.42			C
50	MOTA	7037	CG	LEU		63	•	12.548	83.387	11.771		34.55			C
	MOTA	7039		LEU		63		12.847	82.271	12.775		36.00			C
	ATOM	7043	CD2	FEU		63		13.742	83.634	10.972		36.18			C
	MOTA	7047	С	LEU	·B	- 63			83.913	9.112		45.11			C
	MOTA	7048	0	LEU		63		10.388	83.773	8.099		51.74			0
55	MOTA	7049	N	ARG		64		8.407	83.778	9.132		45.09			N
	MOTA	7051	CA	ARG	В	. 64		7.627	83.437	7.918		45.81			, C
	MOTA	7053	CB	ARG		64		7.621	84.590	6.932		42.03			C
	MOTA	7056	CG	ARG		64	•	8.317		7.448		48.52			C
	MOTA	7059	CD	ARG		64		7.647				42.44			C
60	MOTA	7062		ARG		64	· ·					45.11			N
	MOTA	7064	CZ	ARG	В	64		9.098	88.601	5.721	1.00	47.61			С

5	MOTA	7065	NH1.	ARG B	64		9.754	89.057	6.786		49.17				N
	MOTA	7068	NH2	ARG B	64		9.431	89.044	4.531						N
	MOTA	7071	С	ARG E	64		8.161	82.208	7.176		48.40				Ċ
	ATOM -	7072	0	ARG E	64		8.654	82.321	6.041		50.59				0
	ATOM	7073	N	LYS E	65		8.050	81.058	7.832		44.70				N
10	MOTA	7075	CA	LYS E	65		8.589	79.783	7.378	1.00	42.44				С
	ATOM	7077	CB	LYS E	65		10.110	79.799	7.680	1.00	42.17				С
•	ATOM	7080	CG	LYS E	65	•	11.080	78.794	6.970		46.99				С
	MOTA	7083	CD	LYS E	3 65		12.568	78.665	7.710	1.00	41.67				С
	ATOM	7086	CE	LYS E	65		13.207	80.010	8.378	1.00	31.79				C
15	ATOM	7089	NZ	LYS E	65		14.690	79.980	8.772	1.00	. 2.00				N
	ATOM	7093		LYS E		•	7.817	78.802	8.271		40.97				С
	ATOM	7094		LYS E	3 65		7.650	79.069	9.459		39.90		•		0
	ATOM	7095		GLY E			7.299	77.707	7.711	1.00	45.11				N
•	ATOM	7097		GLY E			6.632	76.656	8.487	1.00	37.19	•			С
20.	ATOM	7100		GLY E	3 66		7.643	75.541	8.684	1.00	43.52				С
- , •.	ATOM	7101		GLY E			8.638	75.469	7.970	1.00	43.64		:		0
	ATOM	7102		VAL E			7.398	.74.674	9.652	1.00	48.15				N
	ATOM	7104		VAL E			8.300	73.575	9.969	1.00	47.91				С
	ATOM	7106		VAL E	3 67		9.347	74.093	10.970	1.00	46.06				С
25	ATOM	7108		VAL E	3 67		8.684	74.740	12.148	1.00	53.01				С
	ATOM	7112		VAL E			10.242	73.023	11.460	1.00	45.35				С
	ATOM	7116	C	VAL E			7.531	72.375	10.546	1.00	48.93				С
	ATOM	7117	0	VAL E			6.604	72.553	11.306	1.00	50.43			-	0
	ATOM	7118	N	TYR F				71.159	10.173	1.00	54.33				N
30	MOTA	7120	CA	TYR E			7.307	69.912	10.681	1.00	54.23				C.
•	ATOM	7122	CB	TYR E			6.674	69.180	9.496	1.00	58.61				С
	ATOM	7125	CG	TYR F			6.194	67.743	9.740	1.00	62.41				С
	ATOM	7126	CD1	TYR F	3 68		5.151	67.465	10.624	1.00	65.98				C.
	ATOM	7128	CE1	TYR E	3 68		4.709	66.183	10.833		65.58				С
35	ATOM	7130	CZ	TYR F	B 68.		5.303	65.145	10.156	1.00	70.65				С
	MOTA	7131	OH	TYR F	B 68		4.874	63.855	10.350	1.00	76.70				0
	ATOM	7133	CE2	TYR F			6.330	65.379	9.274		68.48				С
	ATOM'	7135	CD2	TYR I	B 68		6.766	66.677	9.067	1.00	68.01				С
	ATOM	7137	С	TYR E			8.354	68.969	11.289	1.00	52.15				С
40	MOTA	7138	0	TYR I	B 68		9.446	68.840	10.735	1.00	51.11				0
	ATOM	7139	N	VAL I	В 69		8.028	68.308	12.407	1.00	48.81				N
	ATOM	7141	CA	VAL 1	В 69		8,931	67.350	13.043	1.00	41.24				С
	MOTA	7143	CB	VAL I	В 69		9.433	67.888	14.381	1.00	46.72				С
	ATOM	7145	CG1	VAL I	в 69		10.525	66.959	14.976	1.00	50.12				С
45	MOTA	7149	CG2	VAL I	B 69		9.951	69.297	14.276		44.49				С
	ATOM	7153	С	VAL :	В 69		8.254	66.073	13.454	1.00	42.06			•	С
	ATOM	7154	0	VAL	в 69		7.427	66.130	14.335	1.00	49.53				0
	MOTA	7155	N	PRO 1	в 70		8.562	64.923	12.851		44.13				N
	ATOM	7156	CA	PRO I			8.124	63.637	13.369	.1.00	40.92				С
50	ATOM .	7158	CB	PRO I			8.103	62.804	12.106	1.00	42.89				С
	ATOM	7161	CG	PRO 1			9.343	63.146	11.506	1.00	41.09				С
	ATOM		· CD	PRO 1	в 70		9.306	64.697	11.594	1.00	47.61				С
•	MOTA	7167	C	PRO-			9.149	62.940	14.268	1.00	49.11				С
	ATOM	.7168	0	PRO 1			10.376	62.995	14.009	1.00	49.67		. •		0
55	ATOM	7169	N	TYR			8.645	62.251	15.290	1.00	50.47		•		N
٠.	ATOM	7171	CA	TYR			9.476	61.426	16.149	1.00	53.44				С
	ATOM	7173	CB	TYR			9.170	61.786	17.587	1.00	53.95				С
	MOTA	7176	CG	TYR			9.281	63.268	17.848	1.00	54.07		•		С
	MOTA	7177		TYR			10.380	63.799	18.509		54.07				С
60	ATOM	7179		TYR			10.474	65.154	18.746		54.76				С
~	ATOM	7181	. CZ	TYR			9.475	65.989	18.322		49.10				С
	111011			~							· -				

_		7100	011	TYR	De	71		9.564	67.326	18.547	1.00 49.20			0
5	ATOM	7182		TYR		71		8.397	65.494	17.673	1.00 52.91			С
	MOTA	7184		TYR		71		8.299	64.135	17.437	1.00 55.62			С
	MOTA	7186				71		9.220	59.920	15.888	1.00 57.24			С
	MOTA	7188		TYR				8.666	59.564	14.848	1.00 61.01			0
	MOTA	7189	0	TYR		71			59.045	16.816	1.00 56.65			N
10	MOTA	7190	N	THR		72		9.633	57.601	16.757	1.00 49.69			С
	MOTA	7192	CA	THR		72		9.338		17.843	1.00 45.99			С
	MOTA	7194	CB	THR		72		10.143	56.812	17.485	1.00 41.99			0
	MOTA	7196		THR		72		11.515	56.708		1.00 48.51			C
	MOTA	7198	CG2	THR		72		9.736	55.355	17.907	1.00 40.31			C
15	ATOM	7202	С	THR		72		7.843	57.406	17.025	1.00 51.02			ō
	MOTA	7203	0	THR	В	72		7.208	56.549	16.431				N
	ATOM	7204	N	GLN	В	73		7.303	58.198	17.946	1.00 48.27			, C
	MOTA	7206	CA	GLN	В	73		5.875	58.203	18.263	1.00 48.31			Ċ
•	ATOM	7208	CB	GLN	В	73			57.409	19.545	1.00 51.35			C
. 20	ATOM	.7211	CG	GLN	В	73		5.749	55.888	19.423	1.00 56.02			
. 20	MOTA	7214	CD	GLN		73		4.857	55.255	18.344	1.00 61.90			C
	ATOM	7215		GLN		73		3.792	55.792	18.018	1.00 68.29			0
	ATOM	7216		GLN		73		5.295	54.124	17.783	1.00 62.95			N
	ATOM	7219	С	GLN		73		5.437	59.654	18.470	1.00 49.42			C
25	ATOM	7220	ŏ	GLN		73		5.747	60.278	19.508	1.00 46.54			0
23	MOTA	7221	N	GLY		.74		4.722	60.214	17.499	1.00 48.91			N
	ATOM	7223	CA	GLY		74		4.305	61.606	17.608	1.00 49.47			С
		7226	C.	GLY		74		4.933	62.541	16:584	1.00 50.49		•	С
	ATOM	7227	o	GLY		74		5.998	62.255	16.005	1.00 50.02			0-
20	ATOM	7228	N .	LYS		75		4.266	63.674	16.375	1.00 50.53		•	N
30	ATOM		CA	LYS		75		4.660	64.627	15.342	1.00 52.28			C
	MOTA	7230		LYS		75		4.490	63.974	13.978	1.00 54.30	•		С
	ATOM	7232	CB	LYS		75		3.047	63.970	13.545	1.00 57.04			С
	MOTA	7235	CG			75 75		2.877	63.711	12.065	1.00 62.75			С
	MOTA	7238	CD	LYS		75		3.286	62.309	11,659	1.00 69.74			С
35	MOTA	7241	CE	LYS		75		3.245	62.144	10.151	1.00 75.75			N
	MOTA	7244	NZ	LYS				3.767	65.863	15.374	1.00 48.92			,C
	MOTA	7248	C	LYS		75		2.624	65.773		1.00 50.04			. O
	MOTA	7249	0	LYS		75	•		67.005	14.939	1.00 47.21			N
	MOTA	7250	N	TRP		76		4.288	68.264	14.876	1.00 45.93			С
40	MOTA	7252	CA.			76		3.529	69.023	16.212	1.00 44.91			С
	ATOM	7254	CB	TRP		76		3.623			1.00 44.21			C
	MOTA	7257	CG	TRP		76		5.006	69.104	17.578	1.00 48.52			C
	MOTA	7258		TRP		76		5.635	68.312		1.00 44.12			N
	MOTA	7260		TRP		76		6.950	68.697	17.720	1.00 40.53			C
45	MOTA	7262		2 TRE		76		7.190		16.878			•	Ċ
	MOTA	7263		2 TRE		76		5.985		16.194	1.00 46.96			c.
	ATOM	7264	ÇE:	3 TRE	B	76		5,967			1.00 44.10			C
	MOTA	7266	CZ:	3 TRE	В	76		7.090			1.00 33.58			_
	ATOM	7268	CH:	2 TRE	P B	76		8.269			1.00 44.67			C
50	ATOM	7270	CZ	2 TRE	? B	76		8.324			1.00 38.84			C
50	ATOM	7272		TRE		76		4.014	69.191	13.734				-C
	MOTA	7273		TRE		76		5.038	68.975					0
	ATOM	7274		GLU		77		3.263	70.251	13.522				. · N
		7276				77		3.588		12.483	1.00 54.19			C
55	MOTA	7278				77		2.687			1.00 56.34			C
	MOTA				JB			2.928						С
	ATOM	7281 7284						3.069			•			С
	MOTA			1 GL				2.692						0
	MOTA	7285		2 GL				3.577						0
	ATOM	7286						3.390					•	C
60	ATOM	7287			UB			2.470						0
	ATOM	7288	0	GTI	U B	77		2.470						

5	MOTA	7289	N	GLY E	3 7	8	4.249	73.495	12.906	1.00 39.02		N
	MOTA	7291	CA	GLY F	3 7	8	4.116	74.794	13.527	1.00 38.17		,C
•	MOTA	7294	С	GLY F	37	8	4.560	75.872	12.574	1.00 41.86		С
	ATOM .	7295	0	GLY F		8	4.622	75.629	11.360	1.00 42.61		0
	MOTA	7296	N	GLU I	3 7	9	4.865	77.040	13.150	1.00 40.98	•	И
10	MOTA	7298	CA	GLU I	3 7	9	5.353	78.217	12.458	1.00 40.07		C
	MOTA	7300	CB	GLU I	37	9	4.182	79.179	12.341	1.00 45.01		c.
	ATOM	7303	CG	GLU I	3 7	9	3.271	78.881	11.161	1.00 48.35		C
	MOTA	7306	CD	GLU I	3 7	9	1.879	79.445	11.376	1.00 59.96	•	С
	ATOM	7307	OE1	GLU I	3 7	9	1.026	79.356	10.435	1.00 58.74		. 0
15	ATOM	7308	OE2	GLU I	3 7	9	1.656	79.975	12.506	1.00 62.96		Ó
	ATOM	7309	С	GLU I	3 · 7	9	6.534	78.904	13.206	1.00 39.29		C
	ATOM	7310	0	GLU I	3 7	9	6.387	79.304	14.373	1.00 42.71		0
	ATOM	7311	N	LEU I	3 8	0	7.685	79.057	12.520	1.00 40.28		N
•	ATOM	7313	CA	LEU !	3 8	80	8.955	79.568	13.102	1.00 36.41		С
20	ATOM	7315	СВ	LEU I	B 8	30	10.154	79.219	12.177	1.00 36.64		С
	ATOM	7318	CG	LEU I	B: 8	30	10.738	77.781	12.076	1.00 37.91		C
	ATOM	7320		LEU I	в 8	30	11.526	77.548	10.745	1.00 39.77		С
	ATOM	7324		LEU I		30	11.649	77.344	13.193	1.00 36.07		С
	ATOM	7328	С	LEU		30	8.966	81.088	13.467	1.00 33.54		С
25	ATOM	7329	0	LEU :		30	8.254	81.878	12.905	1.00 32.98		0
23	ATOM	7330	N	GLY		31	9.775	81.482	14.431	1.00 32.51		N
	ATOM	7332	CA	GLY		31	. 9.853	82.869	14.860	1.00 36.03	**	С
•	ATOM	7335	С	GLY		31	11.029	82.934	15.848	1.00 42.04		С
	ATOM	7336	0	GLY		31	11.757	81.938	15.970	1.00 29.06		0
30	ATOM	7337	N	THR		32	11.223	84.089	16.504	1.00 41.12	•	N
50	ATOM	7339	ÇA	THR		32	12.122	84.225	17.659	1.00 44.53		C
٠	ATOM	7341	CB	THR		32	13.486	84.776	17.289	1.00 41.56		С
	ATOM	7343		THR		32	13.438	86.212	17.236	1.00 37.05		0
	ATOM	7345		THR		82	13.898	84.298	15.882	1.00 44.94	•	C
35	ATOM	7349	C	THR		82	11.512	85.157	18.726	1.00 47.70		С
<i>ک</i> ,ک	ATOM	7350	ō	THR		82	10.689	86.007	18.424	1.00 48.47	•	O.
•	ATOM	7351	N	ASP		83	11.949	84.980	19.971	1.00 49.65		N
•	ATOM	7353	CA	ASP		83	11.536	85.805	21.078	1.00 43.80		С
	ATOM	7355	CB	ASP		83	10.137	85.412	21.497	1.00 45.31		С
40	ATOM	7358	CG	ASP	В	83	9.416	86.517	22.208	1.00 48.10		С
	ATOM	7359		ASP		83	10.063	87.357	22.873	1.00 43.35		0
	ATOM	7360		ASP		83	8.174	86.617	22.144	1.00 55.68		0
	ATOM	7361	С	ASP		83	12.515	85.545	22.220	1.00 44.30		С
	ATOM	7362	0	ASP		83	13.317	84.618	22.164	1.00 42.87		0
45	ATOM	7363	N	LEU	В	84	12.431	86.359	23.264	1.00 44.69		N
	MOTA	7365	CA	LEU	В	84	13.305	86.237	24.412	1.00 44.31		С
	ATOM	7367	CB	LEU	В	84	13.298	87.556	25.184	1.00 42.41		С
	ATOM	7370		LEU	В	84	14.000	88.765	24.573	1.00 46.49		С
	ATOM	7372		LEU		84	14.187	89.925	25.584	1.00 45.21		С
50	ATOM	737.6		LEU		84	15.355	88.390	23.988	1.00 47.47		C
30	ATOM	7380	C	LEU		84	12.880	85.069	25.317	1.00 43.92		C
	ATOM	7381	ō	LEU		84	11.702	84.796	25.459	1.00 43.23		0
	ATOM		N	VAL		85	13.859		25.939	1.00 48.76		N
	ATOM	7384	CA	VAL		85		83.210	26.747	1.00 48.52		С
55	ATOM	7386	CB	VAL		85	13.957	81.977	25.854	1.00 49.65		C
,	ATOM	7388		VAL		85		80.668	26.519	1.00 54.85		C
	ATOM	7392		VAL		85		82.099	24.546			С
	ATOM	7396		VAL		85		83.123	28.044	1.00 48.30		С
	ATOM	7397	ŏ	VAL		85		83.170	27.981			0
60	ATOM	7398		SER		86		83.000	29.206			N
JU	ATOM	7400		SER		86		82.778	30.497			С
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55
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                       TYR B 123
                                      25.038
                                               67..830
                                                       18.578
                                                               1.00 50.51
      ATOM
             7959
                   CG
                                                               1.00 52.07
                                               66.616
                                                       19.214
                   CD1 TYR B 123
                                       24.905
      MOTA
             7960
                                                       20.268
                                                               1.00 56.08
                       TYR B 123
                                       25.759
                                               66.249
             7962
                   CE1
      MOTA
                                                       20.679 1.00 57.64
                       TYR B 123
                                       26.759
                                               67.115
                   CZ
             7964
      ATOM
                                                       21.710 1.00 62.04
                       TYR B 123
                                       27.589
                                               66.754
             7965
                   OH
      MOTA
60
                                                       20.054 1.00 58.63
                                       26.917
                                               68.341
      ATOM
             7967
                   CE2 TYR B 123
```

5	MOTA	7969	CD2	TYR	B 123	26.051	68.692	19.001	1.00 56.37		С
Ľ,	ATOM	7971	С	TYR I	B 123	21.979	69.223	16.661	1.00 43.80		. C
	ATOM	7972	0	TYR I	B 123	20.957	68.637	16.350	1.00 50.79	١	0
	MOTA	7973	N		B 124	22.477	70.250	15.982	1.00 43.43	;	N
	MOTA	7975	CA.		B 124	21.793	70.841	14.838	1.00 43.69	1	С
10	MOTA	7977	CB		B 124	22.566	72.036	14.319	1.00 46.07	•	,C
•	MOTA	7981	С		B 124	21.612	69.869	13.717	1.00 42.56	i	C
	ATOM	7982	0	ALA I	B 124	20.594	69.882	13.067	1.00 42.47	1	0
	ATOM	7983	N	GLU I	B 125	22.582	69.006	13.476	1.00 44.82	÷ .	N
	MOTA	7985	CA		В 125	22.469	68.163	12.296	1.00 47.99	·	С
15	MOTA	7987	CB		B 125	23.515	67.059	12.235	1.00 49.37		C
	MOTA	7990	. CG		B 125	22.957	65.812	11.577	1.00 57.34		С
	ATOM	7993	CD.		B 125	23.551	65.493	10.224	1.00 64.77		С
	ATOM	7994		GLU I		24.491	64.674	10.186	1.00 71.72	•	0
	ATOM	7995		GLU I		23.068	66.040	9.201	1.00 74.39		0
20	ATOM	7996	С		3 125	21.107	67.553	12.132	1.00 44.92	•	С
	ATOM	7997	0		3 125	20.708	67.270	11.008	1.00 47.91		0
	MOTA	7998	N		3 126	20.381	67.329	13.219	1.00 43.01		N
	ATOM	8000	CA		3 126	19.116	66.641	13.067	1.00 40.58		С
	ATOM	8002	CB		3 126	19.078	65.412	13.969	1.00 39.84		С
25	ATOM	8004		ILE E		18.870	65.776	15.413	1.00 43.52		С
	MOTA	8007		ILE E		18.662	64.549	16.288	1.00 44.92		C
•	· ATOM	8011		ILE E		20.372	64.751	13.908	1.00 40.38		С
	ATOM	8015	C		3 126	17.962	67.565	13.315	1.00 42.42		С
20	ATOM	8016	0		3 126	16.823	67.138	13.565	1.00 40.90		0
30	ATOM	8017	N		3 127	18.250	68.853	13.236	1.00 42.86		N
	MOTA	8019	CA		3 127	17.202	69.836	13.404	1.00 42.99		С
	ATOM	8021	CB		3 127	17.753	71.130	13.922	1.00 44.98		C
	ATOM	8025	C		3 127	16.525	70.059	12.091	1.00 41.47		С
25	ATOM	8026	0 .		3 127	17.105	69.882	11.050	1.00 39.97		0
35	ATOM	8027	N		3 128	15.272	70.444	12.165	1.00 44.79		N
	MOTA	8029	CA	ARG I		14.517	70.755	10.990	1.00 43.13		. С
	ATOM	8031	CB		3 128	13.282	69.894	10.960	1.00 42.01		С
	ATOM	8034	CG	ARG I		13.574	68.400	11.101	1.00 49.12		С
40	ATOM	8037	CD		3 128	13.536	67.609	9.795	1.00 52.69		С
40	ATOM	8040	NE		3 128	13.330	66.174	10.019	1.00 58.75		N
	ATOM	8042 8043	CZ		3 128	12.511	65.403	9.306	1.00 61.67		C
	ATOM ATOM	8045		ARG E		11.809	65.915	8.308	1.00 58.06		N
	ATOM	8049	C	ARG E		12.396	64.110	9.592	1.00 62.03		N
45	ATOM	8050	0.	ARG E		14.154	72.208	11.134	1.00 41.86		C
- 45	ATOM	8051	N.	PRO E		14.131	72.729	12.258	1.00 39.07		0
	ATOM	8052		PRO E		13.883 13.958	72.863 72.233	10.013	1.00 42.22		N
	AŢOM	8054		PRO E		13.390	73.274	8.694	1.00 43.56		C
•	MOTA	8057	CG		129	12.704	74.240	7.755	1.00 45.93		C
50 -	ATOM	. 8060	CD		3 129		74.249	8.633	1.00 47.55		C
50	ATOM	8063	C	PRO E		13.465 15.348	74.266	9.924	1.00 43.06		· C
	ATOM	8064	0	PRO E		15.524	71.893	8.290	1.00 45.94		C
	ATOM	8065	N ·	ASP E			71.066	7.396	1.00 49.70		0
	ATOM	8067	CA	ASP E		16.340 17.715	72.488	8.929	1.00 51.65		N
55	ATOM	8069	CB	ASP E		18.119	72.086 72.654	8.642	1.00 53.34		C
33	ATOM	8072		ASP E		18.119		7.330	1.00 55.91		C.
	ATOM	8073		ASP E			74.138	7.387	1.00 61.07		C
	ATOM	8074		ASP E		17.510 18.856	74.791 74.738	6.545	1.00 72.80		0
	ATOM	8075	C	ASP E		18.748	72.613	8.265	1.00 52.07		0
60	ATOM	8076		ASP E		18.515	73.579	9.600	1.00 55.45		C.
00	ATOM	8077	И.	ASP E		19.918	71.989	10.342	1.00 58.60		. 0
	WIOU		7.4	nor E	121	19.910	11.989	9.529	1.00 53.37		N

5	ATOM	8079	CA	ASP E	3 131		21.056	72.356	10.347	1.00 52				C
•	ATOM	8081	CB	ASP E	3 131		22.321	71.615	9.849	1.00 56				C
	ATOM	8084	CG	ASP E	3.131		22.898	72.170	8.499	1.00 67				С
	ATOM	8085	OD1	ASP E	3 131		22.369	73.164	7.913	1.00 71				0
	ATOM	8086	OD2	ASP F	3 131		23.911	71.651	7.950	1.00 67				Ö
10	ATOM	8087	С	ASP F	3 131		21.294	73.855	10.486	1.00 47				C
	MOTA	8088	0	ASP I	3 131		22.103	74.261	11.276	1.00 55				0
	ATOM	8089	N	SER I	3 132		20.599	74.692	9.743	1.00 49				N
	ATOM	8091	CA	SER I	3 132		20.799	76.144	9.863	1.00 51				C
	MOTA	8093	СВ		B 132		20.431	76.880	8.576	1.00 56				С
15	MOTA	8096	OG	SER !	B 132		19.064	77.316	8.672	1.00 56				0
10	ATOM	8098	C .		В 132.		19.910	76.773	10.877	1.00 48				С
	ATOM	8099	0	SER	B 132		19.967	77.966	11.030	1.00 48				0
	ATOM	8100	N	LEU !	B 133.		19.044	75.996	11.514	1.00 51				N
•	ATOM	8102	CA		В 133		18.210	76.511	12.594	1.00 48				C
20	ATOM	8104	СВ	LEU !	B 133		16.784	75.967	12.530	1.00 50				С
	ATOM	8107	CG	LEU	В 133		15.867	76.770	13.479	1.00 50				C
	ATOM	8109	CD1	LEU	в 133		15.291	77.914	12.692	1.00 51				C
	ATOM	8113	CD2	LEU	в 133		14.749	75.979	14.133	1.00 46				c
٠.	ATOM	8117	C	LEU	в 133		18.841	76.165	13.947	1.00 48				C
25	ATOM	8118	0	LEU	B 133		18.549	75.164	14.561	1.00 55				0
	ATOM	8119	Ν.	GLU	B 134		19.728	77.021	14.398	1.00 51				N
	ATOM	8121	CA	GLU	B 134		20.411	76.871	15.673	1.00 49				C
	ATOM	8123	CB	GLU	B 134		21.132	78.206	15.930	1.00 52				C
	ATOM	8126	CG	GLU	B 134		.21.942	78.394		1.00 57				C
30	ATOM .	8129	CD	GLU	B 134	·	22.920	79.568	17.051	1.00 62				C
50	ATOM	8130	OE1	GLU	B 134		23.903	79.441	16.281	1.00 65				0
	ATOM	8131	OE2	GLU	B 134		22.717	80.622		1.00 63				0
	ATOM	8132	С		В 134		19.462	76.499	16.822	1.00 46				С
	MOTA	8133	ο.	GLU	B 134		18.509	77.230	17.070	1.00 40				0
35	MOTA	8134	N	PRO	B. 135		19.735	75.368	17.494	1.00 39				N
-	ATOM	8135	ĊA	PRO.	B 135		19.040	74.917	18.710	1.00 40				С
	ATOM	8137	СВ	PRO	B 135		19.597	73.515	18.944	1.00 39				C
•	ATOM	8140	CG	PRO	B 135		20.409	73.187	17.783	1.00 40				С
	MOTA	8143	CD	PRO	в 135		20.750	74.409	17.082	1.00 43				С
40	ATOM	8146	С		B 135		19.301	75.722	19.982					C
	MOTA	8147	0	PRO	В 135		20.327	76.366	20.169	1.00 43				0
	ATOM	8148	N	PHE	B-136		18.361	75.638	20.906	1.00 4				N
	MOTA	8150.	CA	PHE	B 136		18.396	76.470	22.119	1.00 4			•	C
	MOTA	8152	CB	PHE	B 136		17.279	76.100	23.088	1.00 4				C
45	MOTA	8155	CG	PHE	B 136		17.309	76.929	24.293	1.00 3				C
	ATOM	8156			B 136		16.639		24.334	1.00 4				c
	MOTA	· 8158	CE1	PHE	B 136		16.683			1.00 4				c
	MOTA	8160	CZ	PHE	B 136		17.417	78.488	26.517	1.00 4				
	MOTA	· 8162			B 136		18.113			1.00 4				C,
50	MOTA	8164	CD2	PHE	B 136		18.056							C
	MOTA	8166	С	PHE	В 136		. 19.672							C
	MOTA	8167	0		В 136		20.091							0
	MOTA	8168	N	PHE	B 137		20.282							N
	MOTA	8170	CA	PHE	B 137		21.496					•		C
55	ATOM	8172	CB		B 137		21.819							C
•	ATOM	8175	CG		В 137		22.697							C
	ATOM	8176			В 137		22.194							C
	ATOM	8178	CE		B 137		23.015							C
	ATOM	8180	CZ		B 137		24.338							C
60	ATOM	8182	CE		B 137		24.842						•	C
	MOTA	8184	CD	2 PHE	B 137		24.041	73.575	25.394	1.00 4	5.95			С

5	MOTA	8186	С	PHE B 1	L 37	22.696	75.938	23.216	1.00	43.32			С
٠		·· 8187		PHE B		23.468	76.599	23.887	1.00	42.97			0
			N	ASP B		22.843	75.783	21.895	1.00	44.54	•	٠.	N
	MOTA	8188		ASP B		23.891	76.481		1.00	37.01			С
	MOTA	8190	CA	ASP B		23.736	76.253	19.706		35.76			Ç
	MOTA	8192	CB				74.993	19.282		41.96			Ċ
10	MOTA	8195	CG	ASP B		24.247	75.024	18.467		61.10			0
	MOTA	8196		ASP B		25.187				56.89			ō
	MOTA	8197	OD2	ASP B		23.796	73.908	19.672		43.61			Ċ
	MOTA	8198	С	ASP B		23.788	77.995	21.316				•	ő
	MOTA	8199	0	ASP B		24.743	78.650	21.697		47.84			N
15	MOTA	8200	N	SER B	139	22.626	78.554	20.991		46.65			C
	MOTA	8202	CA	SER B		22.433	79.979	21.115		48.26			C
	MOTA	8204	CB	SER B	139	21.004	80.383	20.742		51.54			
	MOTA	8207	OG	SER B	139	20.647	79.872			51.53			0
•	MOTA	8209	С	SER B	139	22.691	80.372	22.526		48.43			С
20	MOTA	8210	0	SER B		23.245	81.423	22.774		49.51			0
20	ATOM	8211	N	LEU B		22.286	79.537	23.470		52.62			N
	ATOM	8213	CA	LEU B		22.480	79.895	24.874		56.48			С
	ATOM	8215	CB	LEU B		21.930	78.831	25.813		56.51			·C
	ATOM	8218	CG	LEU B		22.375	79.194	27.234	1.00	54.72			С
25		8220		LEU B		21.590	80.369		1.00	55.46			. c
23	ATOM	8224		LEU B		22.222	78.095	28.210	1.00	57.48		•	С
	ATOM		C	LEU B		23.955	80.086			57.93			C
	ATOM	8228		LEU B		24.333	81.037	25.897		59.89			.0
	ATOM	8229	0	VAL B		24.793	79.168	24.751		55.68			N
20	MOTA	8230	N	VAL B			.79.300	25.021		54.58			С
30	MOTA	8232	CA	VAL B		26.883	78.025	24.692		58.69			C
	MOTA	8234	CB	VAL B		28.370	78.251	24.440		58.03			С
	ATOM	8236				26.664	77.039			61.23			С
	ATOM	8240		.VAL B		26.822	80.452	24.243		57.01			С
0.5	MOTA	8244	C	VAL B		27.587	81.229	24.817		58.33			0
35	MOTA	8245	0	VAL B		26.517	80.585	22.948		54.66			N
•	ATOM	8246	N	LYS B		27.109	81.677	22.188		51.01			С
	ATOM	8248	CA	LYS B		26.710	81.694	20.673		47.84			С
	MOTA	8250	CB	LYS B		27.455	80.681	19.723		48.68			С
40	ATOM	8253	CG	LYS B		26.743	80.426	18.329		54.09			С
40	MOTA	8256	CD	LYS B			79.184	17.438		59.89			С
	MOTA	8259	CE	LYS B		27.275	77.779	17.577		63.41			N
	ATOM	8262	NZ	LYS B		26.633	82.966	22.952		49.96	•		C
	ATOM	8266	С	LYS B		26.755		23.156		61.21			ō
	ATOM	8267	0	LYS B		27.616		23.130		50.78			N
45	MOTA	8268	N	GLN B		25.521	83.104			49.37			C
	MOTA	8270	CA	GLN B		24.976	84.369	24.029	-	45.79			Č
	MOTA	8272		GLN B		23.414		23.829		47.31			č
	MOTA	8275	CG	GLN B		22.945							č
	MOTA.	8278		GLN B		21.414	84.810			47.17			ő
5 0 ·	MOTA	8279		L'GLN B		20.610		22.936		50.01			N
	ATOM	8280	NE:	GLN B	143	21,028		20.937		0 42.57			
	ATOM	8283	С	GLN B	143	25.276				0 49.46		•	C
	ATOM	8284	0.	GLN B	143	24.919				0 53.59			0
	ATOM	8285	N	THR B	144	25.887				0 54.02		٠.	
55	ATOM			THR B	144 ·	26.271	84.125			0 56.45			C
	ATOM			THR B		25.218				0 58.45			C
	ATOM			1 THR B	144	25.574			1.0	0 57.95			0
	ATOM			2 THR B		23.847		27.968		0 57.06			C
	ATOM			THR B		27.659		27.925		0 62.87			С
60	MOTA			THR B		28.354		26.977	1.0	0 65.39			0
00	ATOM			HIS B	145	28.091		29.174	1.0	0 65.98			N

5	ATOM	8301	CA	HIS	B 145		29.387	82.706			74.26			C
	MOTA	8303	CB	HIS :	B 145		30.175	83.559	30.474			-		C
	MOTA	8306			B 145		30.447	84.988	30.036		86.80			C
	MOTA	8307			B 145		29.853	86.089	30.629		87.60			N
	MOTA	8309			B 145		30.285	87.194	30.045		87.90			C
10	MOTA	8311			B 145		31.142	86.856	29.099		89.90			N
	MOTA	8313	CD2	HIS	B 145		31.263	85.486	29.073		88.35			С
	MOTA	8315			B 145		29.243	81.228	29.905		71.71			С
	MOTA	8316	0	HIS	B 145		30.212	80.600	30.363		71.89			0
	MOTA	8317	N	VAL	B 146		28.031	80.682	29.754		66.58			N
15	ATOM	8319	CA	VAL	B 146		27.678	79.350	30.230		58.14		•	C
	MOTA	8321	CB ·	VAL	B 146		26.233	79.064	29.905		59.42			С
	ATOM	8323	CG1	VAL	B 146		25.936	77.582	29.997		62.47			C
	ATOM	8327	CG2	VAL	в 146		25.357	79.864	30.838		57.89			C
	ATOM	8331	Ċ	VAL	В 146		28.537	78.328	29.562		54.48			С
20	ATOM	8332	0		B 146		28.531	78.205	28.337		59.51			0
	MOTA	8333	N	PRO	B 147		29.288	77.580	30.359		51.96			N
	ATOM	8334	CA	PRO	B 147		30.138	76.562	29.777		49.03			C.
	MOTA	8336	CB	PRO	B 147		30.757	75.883	30.985		46.35			C.
	MOTA	8339	CG	PRO	в 147		30.725	76.871	32.008		44.84			C
25	MOTA	8342	CD	PRO	B 147		29.404	77.576	31.827		51.63			С
	MOTA	8345	С	PRO	в 147		29.250	75.614	29.019		51.04			С
	ATOM	8346	0	PRO	B 147		28.120	75.312	29.390	• .	56.78			0
•	ATOM	8347	N	ASN	B 148		29.782	75.143	27.923		45.46			N
	ATOM	8349	CA	ASN	B 148	-	29.006	74.373	27.015		41.55			C
30	MOTA	8351	CB	ASN	B· 148		29.683	74.441	25.664		43.45			C
	ATOM.	8354	·CG	ASN	B 148	•	28.986	73.682	24.627		41.45			C
	MOTA	8355			B 148		27.770	73.450	24.682		44.14			0
	MOTA	8356	ND2	ASN	B 148		29.744	73.296	23.627		37.99			N
	MOTA	8359	С		B 148		28.991	72.993	27.538		43.05			C
35	ATOM	8360	0	ASN	B 148		29.608	72.076	26.973		40.55			0
	MOTA	8361	, N		B 149		28.283	72.847	28.648		42.80			N
	MOTA	8363	CA		B 149		28.132		29.273		41.70			C
	ATOM	8365	CB.		B 149		29.275	71.263	30.278		39.84	•	•	C
	MOTA	8368	CG		B 149		29.338	69.945	31.031		41.12			C C
.40	MOTA	8370			B 149		30.675	69.702			39.27			C
	ATOM	8374	CD2		В 149		28.368	69.844	32.185		43.77			C
	MOTA	8378	С		В 149		26.812	71.556	30.000		42.18			o
•	MOTA	8379	0		В 149		26.391	72.623	30.409		48.04			
	MOTA	-8380	N		B 150		26.128	70.428	30:161		37.65			N C
45	MOTA	8382	CA		В 150		24.982	70.422	31.068		39.61			c
	ATOM	8384	CB		B 150		23.718	70.954	30.396	•	40.04			c
	ATOM	8387	CG		в 150		23.235	70.093	29.272		41.92			C
	MOTA	8388			B 150		23.411		27.963		40.21			
	MOTA	8390			B 150		22.976	69.678	26.938		37.50			С
50	MOTA	8392	CZ.		B 150		22.352	68.486			45.37	•		C
	MOTA	8394			B.150		22.165	68.070	28.490		40.66			. C
	MOTA	8396	CD2		B. 150		22.608	68.878	29.526		38.93			C
	ATOM	8398	С		В 150		24.829		31.584		42.19	•		C
	ATOM	8399	0	PHE	B 150		25.195		30.883		41.76			0
55	ATOM	8400	N		B 151		24.321	68.798	32.803		37.28			N
	ATOM	8402	CA		В 151		24.135	67.438	33.313		42.07			C
	ATOM	8404	CB		В 151		25.051		34.517		38.99			C
	MOTA	8407	OG		B 151		25.053				34.21			0
	MOTA	8409	С		В 151		22.671				43.06			C
60	MOTA	8410	0		B 151		21.970				45.97			0
	MOTA	8411	N	LEU	B 152		22.207	65.979	33.719	1.00	40.15			N
		•												

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1.00 40.34
                                                        34.122
                                       20.832 65.747
                      LEU B 152
            8413
                  CA
     ATOM
                                                                 1.00 42.16
                                       19.975 .65.313
                                                        32.938
                  CB
                       LEU B 152
            8415
     MOTA
                                                        31.756
                                                                 1.00 38.97
                                       19.590
                                               66.186
                       LEU B 152
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            8418
                  CG
                                                                                       C
                                                        30.911
                                                                 1.00 40.87
                                       18.685
                                               65.352
                  CD1 LEU B 152
     MOTA
            8420
                                                                                       C
                                                        32.159
                                                                 1.00 38.15
                                       18.885
                                               67.410
                  CD2 LEU B 152
     MOTA
            8424
                                                                 1.00 39.44
                                                                                       C
                       LEU B 152
                                       20.743
                                               64.628
                                                        35.107
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            8428
                  C
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                                                                 1.00 35.13
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     MOTA
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                       GLN B 153
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                                                63.157
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                   CG
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18.981
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                                                        41.126
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     ATOM
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                                                63.238
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                   NE2 GLN B 153
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                                                        37.191
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            8445
                                                63.555
                   С
     ATOM
                                                                 1.00 47.27
                                                                                        0
                                                        37.822
                                                64.327
                       GLN B 153
                                    17.613
20
            8446
                   0
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                                                                                        N
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                                                        36.510
                       LEU B 154
                                       17.803
                                                62.538
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                   N
     ATOM
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                                                62.281
                                                        36.551
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                                       16.364
                       LEU B 154
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     ATOM
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                                                61.599
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             8454
                   CG
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                                                        32.748
                   CD1 LEU B 154
                                                61.588
25
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                                                                                        С
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16.081
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                       LEU B 154
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                                                                 1.00 49.47
                                                         37.707
                                                61.330
                       LEU B 154
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                   С
     MOTA
                                                         37.889
                                                                                        ·O
                                                                 1.00 54.75
                                       16.811
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     ATOM
                                                                 1.00 52.56
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                                                61.606
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     ATOM
                   N
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                                                57.930
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                   CA
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                                                                                        С
                       GLY B 156
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                                                         40.923
                   С
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     ATOM
                                                         41.741
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             8482
                   0
                       GLY B 156
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     ATOM
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                                                                                        N
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                   N
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                       ALA B 157
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                   CB
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                                                         44.426
                                                                  1.00 64.25
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                                                56.114
                       ALA B 157
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             8492
                                                                                        Ň
                                                         42.284
                                                                  1.00 66.93
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                                                55.383
                        GLY B 158
             8493
                   N
      MOTA
                                                                                        С
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                                       9.804
                                                 53.966
             8495
                   CA
                       GLY B 158
45
     MOTA
                                                                                        C
                                                         43.351
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                                                53.537
                                        8.530
                        GLY B 158
     ATOM
             8498
                   С
                                                                                        0
                                        8.531
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                        GLY B 158
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                                                                                        N
                                       7.441
                                                                  1.00.70.60
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                                                                                        С
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50
                   CB
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                        PHE B 159
                                         7.228
                                                 55.397
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                   CD1
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                                                 56.634
      ATOM
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                   CE1
                        PHE B 159
                                       6.751
                                                                                         С
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                                                         46.599
                                                                  1.00 68.53
                    CZ
                        PHE B 159
      MOTA
             8512
                                                                                         С
                                                         45.694
                                                                  1.00 67.06
                                        5.690 ·
                                                 57.631
                        PHE B 159
55
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                    CE2
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                                        5.414
                                                 56.383
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                    CD2 PHE B 159
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      MOTA
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                                                         42.502
                        PHE B 159
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      ATOM
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                        PHE B 159
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                        PRO B 160
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              8520
                    N
      MOTA
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                                         3.361
 60
              8521
                    CA
                        PRO B 160
      ATOM
                                                 54.812
                                                         40.899
                                                                  1.00 72.89
                                       2.102
                        PRO B 160
      MOTA
              8523
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_	2001	0526	CG	PRO B	160		2.325	53.429	41.341	1.00	71.93		• •	С
. 5	MOTA	8526		PRO B			3.218	53.519	42.533		69.92		•.	.C
	MOTA	8529 8532		PRO B			2.959	56.894	41.919	1.00	71.65			С
	MOTA	8533	-	PRO B				57.045	43.136	1.00	72.02			0
	MOTA		-	LEU B			2.703	57.841	41.039	1.00	71.52		٠.	N
10	MOTA	8534		LEU B			2.108	59.104	41.403	1.00	75.59			С
10	ATOM	8536		LEU B			3.160	60.196	41.575	1.00				С
	ATOM	8538		LEU B			4.493	59.938	42.269	1.00	78.23			С
	ATOM	8541		LEU B			5.608	60.398	41.338	1.00	78.97			С
	ATOM	8543		LEU B			4.570	60.663	43.611	1.00	75.00			С
. ~	ATOM	8547		LEU B			1.177	59.500	40.252	1.00	76.43			С
15	ATOM	8551	C	LEU B			1.492	59.322	39.071	1.00	79.99			0
	MOTA	8552	0	GLN B			0.016	60.022	40.584		7526			N
	ATOM	8553	N	GLN B				60.579	39.563	1.00				С
	ATOM	8555	CA	GLN E			-2.266	60.698	40.126	1.00	75.84	•		С
00	MOTA	8557	CB	GLN E			-2.314	61.141	41.592	1.00				С
20	MOTA	8560	CG CD	GLN E		•	-1.628	62.471	41.822	1.00				С
	MOTA	8563		GLN E			-0.588	62.767	41.223	1.00				0
	MOTA	8564		GLN E			-2.203	63.281	42.696	1.00				N
	ATOM	8565		GLN E			-0.290	61.961	39.102	1.00				· C
06	ATOM	8568	С	GLN E		:	0.933	62.153	39.019	1.00				0
25	ATOM	8569	0	GLN E			-1.163	62.919	38.811	1.00	74.89			N
	ATOM	8570	N		3 163		-0.706	64.215	38.347		76.31			С
	ATOM .	8572	CA		3 163		-1.665	64.799	37.275		74.58			· c
	ATOM	8574	CB		3 163		-1.457	66.276	36.955		75.98			С
20	ATOM	8577	CG		3 163		-1.774	66.679	35.491		78.50			С
-30	ATOM	8580	CD OE1		B 163		-2.869	66.428	34.982		73.62			. 0
	MOTA	8581			B 163		-0.797	67.316	34.828		77.14			N
	ATOM	8582			B 163		-0.497	65.139	39.566		78.42			· C
	MOTA	8585	C O		B 163		0.544	65.807	39.667		84.37		•	· · O
25	MOTA	8586 8587	N		B 164		-1.452	65.154	40.501		76.38			N
35	MOTA	8589	CA		B 164		-1.369	66.023	41.690	1.00	73.78			С
	ATOM ATOM	8591	CB		B 164		-2.442	65.635	42.714	1.00	71.78			С
	MOTA	8594	OG		B 164		-2.807	66.743	43.533	1.00	71.79			0
	ATOM	8596	C		B 164		-0.014	65.965	42.395	1.00	76.38			C
40	MOTA	8597	ŏ		B 164		0.467	66.969	42.942	1.00	71.19			0
40	MOTA	8598	N.		B 165		0.590	64.778	42.378	1.00	78.65			N
	ATOM	8600	CA		B 165		1.805	64.521	43.125	1.00	82.23			С
	ATOM	8602	CB		B 165		1.948	63.017	43.344	1.00	86.01			С
•	MOTA	8605	CG		B 165		0.848	62.399	44.201	1.00	88.14			. C
45	ATOM	8608	CD		B 165		1.063	60.911	44.445	1.00	90.26			С
73	ATOM	8609			B 165		2.025	60.560	45.159	1.00	87.30			0
•	ATOM	8610			B 165		0.266	60.089	43.928	1.00	95.66			0
	ATOM	8611	C		B 165		3.053	65.082	42.436	1.00	81.15			С
	ATOM	8612	ŏ		B 165		3.975	•	43.096	1.00	76.40		•	0
50	ATOM	8613	N	VAT.	B 166		3.080		41.111		79.46			, N
50	ATOM	8615	CA		В 166		4.196		40.338	1.00	77.43			С
	ATOM	8617	CB		B 166		4.063			1.00	75.19			. C
		8619			B 166		4.836				77.04			· C
	ATOM	8623			B 166		4.538				74.61			C
55	MOTA	8627	C		B 166		4.353				75.47			C
-55	MOTA		Ö		B 166		5.468				75.66			0
	ATOM	8628 8629	N		B 167		3.259		_		75.60			N
	ATOM	8631	CA		B 167		3.348				75.68	•		С
	MOTA MOTA	8633	CB		B 167		1.977				76.77			С
60		8636			B 167		1.248				80.17			С
60	ATOM	8638			B 167		-0.170				77.26			С
	MOTA	0000	ÇD.	טמע	2 10.									

•	- 001	0642 CD2	2 LEU B 167		2.047	70.399	38.282	1.00	82.87				C
5	ATOM		LEU B 167		3.887	69.644		1.00	73.27.			(С
	ATOM		LEU B 167		4.593	70.643	42.476		69.74			(0
	ATOM	8647 0			3.543	68.848	43.288		73.73			1	N
	MOTA	8648 N	ALA B 168		3.962	69.147	44.636		77.27			(С
	ATOM	8650 CA	ALA B 168			68.585	45.638		75.98				С
10	MOTA	8652 CB	ALA B 168		2.949	68.596	44.921		78.89				С
	MOTA	8656 C	ALA B 168		5.353		45.889		84.58				0
	MOTA	8657 0	ALA B 168		5.995	69.005			76.97				N .
	MOTA	8658 N	SER B 169		5.832	67.688			77.52				C
	MOTA	8660 CA	SER B 169		7.094	67.029	44.373	1.00	80.08				c
15	MOTA	8662 CB	SER B 169		6.858	65.549	44.637						Ö
	MOTA	8665 OG			5.612	65.396	45.312		83.47				c
	ATOM	8667 C	SER B 169		8.122	67.204	43.285		75.54				o
	MOTA	8668 O	SER B 169		7.817	67.604	42.162		69.75				N
•	MOTA	8669 N	VAL B 170		9.355	66.890	43.658		74.47				
20	ATOM	8671 CA	VAL B 170	1	0.511	67.097	42.805		73.73				С
20	ATOM	8673 CB		. 1	1.777	67.421	43.675		72.68				С
	ATOM		1 VAL B 170	1	3.078	67.140	42.959		74.83				С
•	ATOM		2 VAL B 170		1.755	68.881	44.098		72.94				С
	ATOM	8683 · C	VAL B 170		0.654	65.893	41.861		71.65				С
25		8684 0	VAL B 170		9.950	64.866	42.012		75.35				0
23	ATOM	8685 N	GLY B 171	1	1.525	66.035	40.863	1.00	64.10	•			N
	ATOM				1.730	64.987	39.890	1.00	57.27				С
			GLY B 171		3.146	64.918	39.419		52.94				С
	MOTA	8690 C	GLY B 171		3.434	64.116	38.563		50.16				0
20	MOTA	.8691 0			4.024		39.959		48.11				N
30	ATOM	0052			5.412	65.704	39.591		48.37				С
	MOTA	8694 CA			15.975	67.066	39.249		51.80				С
	MOTA	8697 C	GLY B 172		15.357	68.102	39.524		54.56				0
	MOTA	8698 O	GLY B 172			67.063	38.658		48.83				N
	ATOM	8699 พ	SER B 173		17.167	68.288	38.259		43.89				С
35	MOTA	8701 CA			17.796		39.113		42.65		•		С
	MOTA	8703 CE			19.000	68.557	40.373		49.32				Ō
	MOTA	8706 00			18.603	69.033			44.21				Č
	ATOM	8708 C	SER B 173		18.297	68.264	36.864		45.21				ō
	ATOM	8709 0	SER B 173		18.544	67.207	36.273		43.21				N
40	MOTA	8710 N	MET B 174		18.432	69.476	36.356) 43.20) 43.58				c
	MOTA .	8712 C			19.138	69.725	35.148						c
	ATOM	8714 CE			18.184		34.044		43.84				Č
	ATOM	8717 C	S MET B 174		18.971		32.883		46.91				s
	MOTA	8720 SI	D MET B 174		18.074		31.472		53.60				C
45	ATOM	8721 CI	E MET B 174		17.365				56.75				
	MOTA	8725 C	MET B 174.		20.132				0 45.69				С
	ATOM	8726 0	MET B 174		19.721	72.028	35.575		0 45.35				0
•	ATOM	8727 N			21.418	70.577			0 41.84				N
	MOTA	8729 C			22.376		35.853		0 46.48				C,
50		8731 C			23.548			1.0	0 47.95				C
30	MOTA		G1 ILE B 175		23.105			1.0	0 46.56	•			С
•	MOŢA		D1 ILE B 175		22.250				0 46.76				С
	MOTA		G2 ILE B 175		24.168				0 45.43				С
	ATOM				22.986	·	•		0 44.88				С
	MOTA	8744 C			23.615				0 48.63				0
55	ATOM	8745 0							0 51.15				N
	MOTA	8746 N			22.815	11 -			0 51.24				C
	MOTA		A ILE B 176		23.223				0 51.72				C
	MOTA		B ILE B 176		22.198				0 45.30				c
	ATOM		G1 ILE B 176		20.833								č
60	MOTA		D1 ILE B 176		20.454				0 49.64				·C
	ATOM	8759 C	G2 ILE B 176		22.621	75.606	31.139	1.0	0 53.65				C

_		22.62	-	LE B 176		24.558	74.647	33.020	1.00	50.93		(2
5	ATOM	8763 C		LE B 176			75.704	33.620	1.00	52.76	. 4-1	. , (
	MOTA	8764 · O		SLY B 177			74.065	32.413		53.67			
	MOTA	8765 N		SLY B 177		26.921	74.625	32.462	1.00	52.15			
	MOTA	8767 C		GLY B 177		27.839	74.139	33.561		48.67			3
	MOTA	8770 C		GLY B 177		28.832	74.776	33.795		52.76)
10	MOTA	8771 0		SLY B 178		27.538	73.029	34.224		51.24			N
	MOTA	8772 N				28.406	72.536	35.293		51.26			C
	ATOM	8774 C		GLY B 178		28.016	71.184	35.886		52.43			C
	ATOM	8777 C		GLY B 178		27.068	70.577	35.440		59.00		9	Ο,
	ATOM	8778 0		GLY B 178		28.730	70.717	36.903		50.07			N
15	MOTA		•	ILE B 179		28.446		37.512	1.00	45.67			С
	MOTA			ILE B 179		29.610	68.519	37.252		47.32			С
	MOTA			ILE B 179		29.842	68.357	35.761		49.07			С
٠.	MOTA			ILE B 179		31.133	67.633	35.429		45.35			С
	MOTA			ILE B 179		29.350	67.174	37.842		48.87	-		С
20	MOTA	•		ILE B 179		28.271	69.601	39.024		46.31			С
	ATOM	8796 C		ILE B 179		29.115	70.203	39.691		48.40			0
	MOTA	8797 C		ILE B 179		27.199	69:060	39.581		45.06			N
	MOTA	•		ASP B 180			69.265	40.996		46.20			С
	MOTA		CA ·	ASP B 180		26.925 25.489	69.733	41.193		48.62			С
25	MOTA	• • • =		ASP B 180			70.143	42.644		50.85			С
	ATOM			ASP B 180		25.183	71.353	42.922		46.55			0
	MOTA			ASP B 180	•	25.059	69.324	43.579		57.84			Ò
	ATOM			ASP B 180	•	25.034	68.037	41.828		46.31			С
	ATOM	• • • •	C .	ASP B 180		27.169	67.217	41.996		52.16			0
30 -			9	ASP B 180		26.308 28.377	67.942	42.351		51.89			N
	MOTA		N	HIS B 181			66.897	43.277		50.52			С
•	MOTA			HIS B 181		28.831	67.496	44.061		50.18			С
	MOTA		CB	HIS B 181		29.990 31.190	67.731	43.220		60.85			С
	MOTA		CG	HIS B 181			68.400	43.673		67.21			N
35	MOTA			HIS B 181		32.309 33.207		42.704		70.69		•	С
•	MOTA	-		HIS B 181		32.708	67.841	41.639		75.54			N
	ATOM	-		HIS B 181		31.447	67.381	41.936		67.45			С
•	ATOM			HIS B 181		27.858	66.226	44.276		48.76			С
40	ATOM		C	HIS B 181		28.090	65.086			50.74			O.
40	MOTA	- ·	0			26.797	66.891	44.718		47.39			N
	ATOM		N	SER B 182 SER B 182		25.899	66.216			47.06			С
	MOTA		CA .			25.005	67.213			44.50			С
	MOTA		CB	SER B 182 SER B 182	,	24.325	67.978			49.42			0
4.0	MOTA	-	OG.	SER B 182		25.041	65.202			44.21			С
45	ATOM		C	SER B 182		24.473	64.259			42.19			0
	ATOM		0	LEU B 183		24.941	65.377			35.22			N
	ATOM		N.	LEU B 183		24.017	64.548			34.72			С
	ATOM		CA	LEU B 18.		23.541			1.00	37.22			С
-	ATOM		CB	LEU B 18:	,	23.060				0 35.27			С
50	ATOM	8846	CG	LEU B 18		22.723				0 35.13			·C
:	MOTA	8848				21.845				0 39.21			С
	MOTA	8852		LEU B 18		24.581				0 34.54			С
	MOTA	8856	С	LEU B 18		23.893				0 32.68			0
	MOTA	8857	0	LEU B.18						0 40.53			N
55	MOTA	8858	N	TYR B 18		25.814				0 40.17			С
	MOTA	8860	CA	TYR B 18	*± A	26.304				0 42.80			·C
	MOTA	8862	CB	TYR B 18	4 .	26.806				0 39.74			С
	ATOM	8865	CG	TYR B 18	4	28.109 28.111				0 37.66			С
	MOTA	8866	CD	TYR B 18	4					0 37.61			С
60		8868		TYR B 18	4	29.253				0 47.41	•		С
	MOTA	8870	CZ	TYR B 18	*	30.456	, 03.023		~.0				

5	ATOM	8871	ОН	TYR B		-	.576	64.426			55.00			0
	MOTA	8873	CE2	TYR B	184	30	.520	62.236	40.906		43.25			C.
	MOTA	8875	CD2	TYR B	184	29	.322	61.520	41.083		41.71			С
	ATOM	8877	C	TYR B	184	27	.436	60.952	43.634		41.79			С
	MOTA	8878	0	TYR B	184	28	.095	61.684	44.365		46.68			0
10	ATOM	8879	N	THR B	185	27	.686	59.655	43.536		43.21			N
-	ATOM	8881	CA	THR B	185	28	.744	59.045	44.328		44.21			С
:	ATOM	8883	CB	THR B	185	28	1.163	58.164	45.366		44.37			С
	ATOM	8885		THR B	185	27	.282	57.235	44.714		55.13			0
	ATOM	8887	CG2	THR B		27	1.257	58.969	46.275		43.63			С
15	ATOM	8891	С	THR B	185	29	676	58.215	43.499		43.25			С
13	ATOM	8892	0	THR B	185	29	280	57.701	42.428		41.22	. 0		0
	ATOM	8893	N	GLY B		30	.912	58.084	44.009		36.99			N.
	ATOM	8895	CA	GLY B		31	1.934	57.353	43.311		37.15			C
•	ATOM	8898	C	GLY B		32	2.359	58.174	42.111	1.00	39.52			С
20	ATOM	8899	.0	GLY B			1.993	59.309	41.970		41.98			0
20	ATOM	8900	N	SER B		3:	3.106	57.606	41.199		41.91			N
	MOTA	8902	CA	SER B		3:	3.702	58.455	40.213		43.54			С
	ATOM	8904	СВ	SER B			5.132	57.957	39.931	1.00	49.17			С
	ATOM	8907	OG	SER B			5.905	57.864	41.143		51.70			0
25	ATOM	8909	C	SER B			2.906	58.552	38.968	1.00	38.74			С
23	MOTA	8910	ō	SER B			2.171	57.665	38.677	1.00	44.27			0
	ATOM	8911	N	LEU B			3.054	59.649	38.236	1.00	36.60			N
	ATOM	8913	CA	LEU B			2.451	59.779	36.908	1.00	36.77			С
	ATOM	8915	СВ	LEU B			2.452	61.247		1.00	29.29			. C
30	ATOM	8918	CG	LEU B			1.170	62.059	36.695	1.00	26.22			С
. 30	ATOM	8920		LEU B			1.400	63.517	36.419		31.52		•	С
	ATOM	8924		LEU B			0.078	61.647	35.819	1.00	28.00			С
	ATOM	8928	C	LEU B			3.233	59.037	35.839	1.00	37.01			′C
	ATOM	8929	ŏ	LEU B			4.379	59.346	35.689		42.16	٠.		0.
35		8930	N	TRP B			2.622	58.095	35.096	1.00	44.14			N
33	MOTA	8932	CA	TRP B			3.225	57.450	33.888	1.00	40.20			С
	MOTA	8934	CB	TRP B			3.043	55.957	33.873		42.63			С
	MOTA	8937	CG	TRP B			3.929	55.247	34.839		44.06			С
	ATOM	8938	CD1				3.638	54.972	36.099	1.00	38.39			С
40	ATOM ATOM	8940		TRP B			4.685	54.319	36.695		45.18			N
40	ATOM	8942		TRP B			5.687	54.158	35.787	1.00	44.17			C
	ATOM	8943		TRP B			5.248	54.733	34.600	1.00	44.91			С
	ATOM	8944		TRP B			6.102	54.699	33.487	1.00	53.36			С
	ATOM	8946		TRP B			7.351	54.090	33.618	1.00	52.20			С
45		8948		TRP B			7.752	53.528	34.833		50.78			С
43	MOTA	8950		TRP B			6.938	53.549	35.923		50.20			С
	MOTA	8952	C	TRP B			2.610	57.975	32.572		43.79			С
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50	ATOM	8954	N				3.154				39.84			С
50	ATOM	8956	CA	TYR B			34.052				36.42			С
	MOTA	8958	CB	TYR B			33.685				33.81			С
	ATOM	8961	CG				34.442				37.07			С
	ATOM	8962		TYR B			34.111				42.72			С
	ATOM	8964		L TYR B							0 45.10			Ċ
55	ATOM	8966	CZ	TYR B			32.992				53.55			.0
	MOTA	8967	OH	TYR B			32.601				0 30.96			c
	ATOM	8969		2 TYR B			32.255				0 33.25			c
	ATOM	8971		2 TYR E			32.597				0 38.96			c
	MOTA	8973		TYR E			33.386				0 51.45			ő
60	ATOM	8974	0	TYR E			34.524				0 47.13			N
	MOTA	8975	N	THR E	3 191	•	32.312	57.822	28.210	1.0	0 41.17			••

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                      O TYR B 122

N GLU B 200 25.422 CA GLU B 200 25.573 5

CB GLU B 200 25.609 5

CG GLU B 200 25.766 5

CD GLU B 200 26.297 5

OE1 GLU B 200 26.309 OE2 GLU B 200 26.707 C GLU B 200 26.810 O GLU B 200 27.810 N VAL B 201 26.703 CA VAL B 201 27.773 CB VAL B 201 27.773 CB VAL B 201 27.515 CG1 VAL B 201 27.484 CG2 VAL B 201 27.783 O VAL B 201 27.783 O VAL B 201 26.965 28.701
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ILE B 202 28.701
ILE B 202 30.262
ILE B 202 30.075
ILE B 202 31.097
ILE B 202 30.727
ILE B 202 29.052
ILE B 202 29.052
ILE B 202 29.706
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5	ATOM	9201	N	ILE E	3 203	•	28.429	50.423	22.252		42.56			N
	ATOM	9203			3 203		28.259	49.497	23.327	1.00	45.31			C
	ATOM	9205			3 203		26.823	49.150	23.567	1.00	43.41			С
	ATOM	9207			3 203		26.040	50.325	24.088	1.00	41.62			С
	ATOM	9210			3 203		24.600	49.972	24.158	1.00	42.16			С
10		9214			B 203		26.780	48.073	24.599	1.00	44.28			С
10	MOTA	9214			B 203		28.888	48.250	22.866	1.00	49.14	٠.		C
	MOTA	9219			B 203		28.537	47.712	21.806	1.00	47.82			0
	MOTA				B 204		29.782	47.762	23.696		49.32			N
	MOTA	9220			B 204		30.610	46.689	23.294		48.88			C
	ATOM	9222			B 204		31.996	47.004	23.720		45.35			С
15	ATOM	9224			B 204		32.441	48.273	23.012		49.69			C.
	ATOM	9226			B 204		32.055	47.203	25.163		44.93			С
	ATOM	9230				•	30.179	45.382	23.866		51.35			С
	ATOM	9234			B 204		30.565	44.349	23.337		57.30			0
	ATOM	9235			B 204		29.392	45.397	24.941		50.88			N
-20	MOTA	9236			B 205		29.044	44.122	25.568		52.74			С
	ATOM.	9238			B 205			43.498	26.174		52.53			С
	MOTA	9240			B 205		30.299	42.536	27.318		54.44			C
	MOTA	9243			B 205		30.064		27.754		56.13			Č
	ATOM	9246	CD		B 205		31.354	41.863			59.87			N
. 25	ATOM	9249	NE		B 205		31.296	41.266	29.087 29.378		59.78			C.
	MOTA	9251	CZ		В 205		31.742	40.048			58.07			N
	MOTA	9252			B 205		32.275	39.296	28.429		61.85			N
	MOTA	9255			B 205		31.657	39.585	30.618		50.44			C
	ATOM	9258	C.		B 205		27.953	44.177	26.605		60.70			ő
30	MOTA	9259	0		B 205		28.004	44.985	27.512					Ņ
	ATOM	9260	N		B 206		26.972	43.298	26.455		48.83			C
•	ATOM	9262	CA		B 206		25.846	43.189	27.373		48.98			C
	ATOM	9264	CB		в 206		24.544	43.113	26.609		47.56			C
	MOTA	9266	CG1	VAL	B 206		23.429	42.948	27.571		51.41			C
- 35	MOTA	9270	CG2		B 206		24.310	44.358			47.81			C
	ATOM	9274	C		В 206		25.931	41.888	28.204		49.62			
	ATOM	9275	0	VAL	B 206		26.324	40.839	27.707		51.17			0
	MOTA	9276	N		B 207		25.549	41.972	29.466		48.53			И
	MOTA	9278	CA	GLU	B 207		25.511	40.846	30.346		50.25			C
40	MOTA	9280	CB	GLU	B 207		26.588	40.933	31.415		50.16			C
	ATOM	9283	CG	GĻŪ	В 207		27.966	40.533	30.976		49.74			C
	MOTA	9286	CD	GLU	В 207		28.971	40.942	32.003		49.93			С
	ATOM	9287	OE1	GLU	B 207		28.551	41.333	33.115		53.30			0
	ATOM	9288	OE2	GLU	B 207		30.168	40.887	31.697		51.43			0
45	ATOM	9289	С	GLU	B 207		24.194	40.846	31.063		53.82			C
	ATOM	9290	0		B 207		23.625	41.879	31.314		53.60			0
	MOTA	9291	N	ILE	B 208	•	23.715	39.664	31.408		56.66			.N
	ATOM	9293	CA		B 208		22.535	39.565	32.224		54.83			С
	ATOM	9295	СВ		B 208		21.422	38,952	31.434	1.00	55.18			С
50	MOTA	9297			B 208		21.118		30.212		56.27			С
50	ATOM	9300			B 208		20.393		30.503		49.77			. С
		9304			B 208		20.205				57.22			С
	MOTA	9308	C		B 208		22.955		33.429		57.88			С
	ATOM				B 208		23.347		33.302		57.17			0
25	MOTA	9309					22.883		34.603		0 54.93			. N
55	ATOM	9310	N		B 209		23.319		35.835		0 56.25		٠.	C
•	ATOM	9312	CA		B 209		22.270		36.372		0 54.61			c
	ATOM	9314	CB		B 209						0 55.46			č
•	MOTA	9317	CG		B. 209		21.639		38.187		0 50.67			ō
	ATOM	9318			B 209		21.992							Ŋ
60		9319			В 209		20,695		38.189		0 53.95			c
	ATOM	9322	С	ASN	B 209	ı	24.668	38.015	35.668	, I.U	0 52.94			Ŭ

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36.887 36.076 1.00 47.18
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5	MOTA		CB	CYS B	217			44.299	18.997	1.00	74.46			. 5	S .
	MOTA	9437	SG	CYS B		•	28.007	44.565	18.282	1.00	70.29			(3 ·
	MOTA	9438	C	CYS B			27.287	45.509	18.640	1.00	68.93			()
	MOTA	9439	0	CYS B				44.334	17.002	1.00	71.63			1	N
	ATOM	9440	N	LYS B			28.244 27.750		16.014		70.37			. (С
10	MOTA	9442	CA	LYS B					14.611	1.00	71.99				С
	MOTA	9444	CB	LYS B			28.259	44.933	13.943	1 00	76.53				С
	MOTA	9447	CG	LYS B			29.041	46.076	12.496		80.60				С
	MOTA	9450	CD	LYS B			29.452	45.730	11.896		83.08				С
	ATOM .	9453	CE	LYS B			30.493	46.715	12.763		84.11		٠		N
15	MOTA	9456	NZ	LYS B			31.690	46.955	16.063		66.79				C.
	ATOM .	9460	С	LYS B			26.229	45.322			63.62		•		0
	MOTA	9461	0	LYS B			25.578	46.202	15.509		64.08				N
	MOTA	9462	N	GLU B			25.659	44.352	16.743		66.34				C
•	ATOM	9464	CA	GLU B	219		24.222	44.244	16.800	1.00	69.58				c
20	ATOM	9466	CB	GLU B	219		23.839	42.798	17.059		71.88				c
	MOTA	9469	CG	GLU B			24.551	41.798	16.166						C
	ATOM .	9472	CD	GLU B			23.800	41.529	14.875		78.40				Ö
	ATOM	9473	OE1	GLU B	219		22.637	42.002	14.721		72.86				
	ATOM	9474		GLU B			24.389	40.835	14.009		85.55				0
25	ATOM	9475	С	GLU B			23.691	45.065	17.931		65.05				С
23	ATOM	9476	0	GLU B			22.528	45.438	17.961		63.97				0
	MOTA	9477	N	TYR B			24.550	45.342	18.888		65.15				N
	ATOM	9479	CA	TYR B			24.080	45.993	20.070		62.09				C
	ATOM	9481	СВ	TYR E			25.134	45.900	21.179		62.12				C
30	ATOM	9484	CG	TYRE			25.409	44.536	21.845		56.86				C
30	ATOM	9485		TYR E	220		26.716	44.158	22.123		60.11				C
	•	9487	CE1		3 220		27.019	42.952	22.738		59.02				С
	ATOM	9489	CZ	TYR E			26.013	42.097	23.090		60.03				С
	MOTA	9490	OH	TYR E			26.387	40.915	23.694	1.00	65.94				0
25	MOTA	9490		TYR			24.689	42.438	22.840		57.10				С
35	MOTA	9494		TYR			24.396	43.658	22.216		55.80				С
	MOTA	9494	C		3 220		23.817	47.430	19.628		61.17				С
	ATOM	9497	Ö		3 220		22.944	48.103		1.00	64.67				0
	MOTA		N	NCM I	B 221		24.569	47.880	18.628		59.63				N
40	MOTA	9498 9500	CA	ו מכת	B 221		24.486	49.244	18.114	1.00	56.38				С
40	MOTA	9502	CB		B 221		25.865	49.780	18.037	1.00	53.93				С
	ATOM		CG		B 221		26.510	49.843		1.00	51:48				С
	MOTA	9505	CG	L ASN	0 221		26.001	50.434		1.00	51.50	•			0
	MOTA	9506	VD.	2 ASN	D 221		27.686	49.245		1.00	56.63				N
40	ATOM	9507			B 221		23.971			1.00	58.77				С
45	MOTA	9510	C	VCM .	B 221		24.232				59.98				0
	ATOM	9511			B 221		23.235				59.18				N
	ATOM	9512	N		в 222 В 222		22.870				60.10			٠.	С
	ATOM	9514	CA				22.291		•		64.25				·C
	MOTA	9516	CB	TIR	B 222		21.579				65.11				. C
50	MOTA	9519	CG	TYR	B 222		22.008				0 67.45				С
	MOTA	9520	CD	1 TYR	B 222			•			0 68.44				С
	MOTA	9522		1 TYR	B 222		21.356				0 68.04				С
	MOTA	9524	CZ		B 222		20.261	_			0 72.86				0
	MOTA	9525			B 222		19.605				0 72.00 0 65.98				C
55	MOTA	9527	CE	2 TYR	B 222	3	19.814				0 66.41		. •		c
	MOTA	9529	CD	2 TYR	B 222	2	20.470								Č
,	MOTA	9531	C	TYR	B 222	2	21.922				0 57.69				ō
	ATOM	9532		TYR	B 222	2	20.737				0 57.52				N
	ATOM	9533		ASP	B 223	3	22.571				0 58.59				C
60	MOTA	9535		ASP	B 223	3	22.05				0 57.20				· C
7,7	ATOM	9537		ASP	В 223	3	20.51	l 51.264	4 13.178	3 - 1.0	0 62.18	3		•	C
				-									•		

5	ATOM	9540	CG -	ASP B 223		19.929	52.514	12.350	1.00 65.70			С
	ATOM	9541	OD1	ASP B 223 ·		19.045	53.192	12.919	1.00 72.63			0
	ATOM	9542		ASP B 223		20.243	52.884	11.172	1.00 60.60			0
	ATOM	9543	c	ASP B 223		22.694	52.313	14.142	1.00 52.54			С
	MOTA	9544	Ö	ASP B 223		23.514	53.049	13.659	1.00 53.53			0
10		9545	N	LYS B 224		22.364	52.357	15.416	1.00 55.48			N
10	MOTA			LYS B 224		22.905	53.373	16.312	1.00 53.90			C
	ATOM	9547	CA	LYS B 224		22.306	54.743	16.002	1.00 55.04			С
	MOTA	9549	CB	LYS B 224		20.794	54.865	16.179	1.00 52.13	•		C
	MOTA	9552	CG			20.794	56.306	15.817	1.00 47.46			C
	MOTA	9555	CD	LYS B 224				15.312	1.00 47.23			Ċ
15	MOTA		CE	LYS B 224		18.962	56.435		1.00 47.81			Ň
	ATOM	9561	NZ	LYS B 224		18.922	56.181	13.825	1.00 47.31			Ċ
	MOTA	9565	С	LYS B 224		22.640	53.044	17.752		÷		o
	MOTA	9566	0	LYS B 224		22.165	51.982	18.073	1.00 56.88			
•	MOTA	9567	N	SER B 225		22.974	53.966	18.632	1.00 59.75			N
20	MOTA	9569	CA	SER B 225		22.735	53.775	20.046	1.00 58.65			С
	ATOM	9571	CB	SER B 225		23.820	52.902	20.666	1.00 58.31			С
•	ATOM	9574	OG	SER B 225		23.410	51.542	20.653	1.00 64.32			0
	ATOM	9576	c	SER B 225		22.795	55.133	20.625	1.00 51.40			C
	ATOM	9577	0	SER B 225		23.838	55.743	20.585	1.00 52.21			0
25	ATOM	9578	N	ILE B 226		21.681	55.609	21.159	1.00 48.97			N
20	ATOM	9580	CA	ILE B 226		21.652	56.966	21.677	1.00 47.18			С
	ATOM	9582	СВ	ILE B 226	•	20.782	57.870	20.775	1.00 42.41			. C.
	ATOM	9584		ILE B 226		19,421	57.276	20.563	1.00 36.20			С
	ATOM	9587				18.355	58.275	20.220	1.00 36.28			C
30	ATOM	9591		ILE B 226		21.425	58.015	19.433	1.00 45.19			Ċ
30		9595	C	ILE B 226		21.191	57.023	23.126	1.00 45.97			C
	ATOM		o	ILE B 226		20.610	56.051	23.598	1.00 43.09			0
	ATOM	9596		VAL B 227	•	21.491	58.152	23.797	1.00 43.58			N
	ATOM	9597	N	VAL B 227		21.061	58.457	25.177	1.00 -44.91			С
25	ATOM	9599	CA	VAL B 227		22.211	59.070	26.001	1.00 40.77			С
35	ATOM	9601	CB			21.726		27.313	1.00 40.80			C
	MOTA	9603		VAL B 227		23.360	58.096	26.187	1.00 38.82			Ċ
	ATOM	9607		VAL B 227			59.511	25.104	1.00 30.02			Č
	ATOM	9611	С	VAL B 227		19.926		24.596	1.00 40.33			o
	ATOM	9612	0	VAL B 227		20.150			1.00 30.23	•		N
40	MOTA	9613	N	ASP B 228		18.730	59.205	25.624			•	C
	MOTA	9615	CA	ASP B 228		17.565	60.043	25.336	1.00 40.47 1.00 38.92			c
	MOTA	9617	CB	ASP B 228		16.936	59.514	24.036				c
	MOTA	9620	CG	ASP B 228		15.690	60.286	23.615	1.00 45.59			Ö
	ATOM	9621		ASP B 228		15.409	61.367	24.161	1.00 41.67			
45	MOTA	9622	OD2	2 ASP B 228		14.903	59.871	22.744	1.00 55.53			0
•	MOTA	9623	С	ASP B 228		16.512	60.133	26.470	1.00 43.36			C
	MOTA	9624	0	ASP B 228		15.725	59.217	26.694	1.00 38.56			0
	ATOM	9625	N.	SER B 229		16.488			1.00 47.36	•		N.
	ATOM	9627	CA	SER B 229		15.612	61.464	28.310	1.00 47.52			С
50	ATOM	9629	CB	SER B 229		16.147	62.621	29.118	1.00 47.91			С
	ATOM	9632	OG ·			16.818	63.473	28.231	1.00 51.18		٠	0
	ATOM	9634		SER B 229		14.158	61.708	27.934	1.00 49.38			C.
	ATOM	9635	Ō	SER B 229		13.330	61.994	28.798	1.00 54.96			0
	ATOM	9636	N	GLY B 230			61.632	26.644	1.00 48.92		. •	N
55		9638	CA	GLY B 230		12.481	61.753	26.176	1.00 45.57		• •	С
JJ	MOTA		CA	GLY B 230		11.935	60.429	25.637	1.00 48.29			С
	MOTA	9641				10.833	60.372	25.085	1.00 40.94			Ō
	MOTA	9642	0	GLY B 230		12.735		25.785				N
	MOTA	9643	N	THR B 231		12.733						C
~ ^	MOTA	9645	CA	THR B 231								c
60	MOTA	9647	CB	THR B 231		13.349						ő
	MOTA	9649	OG.	1 THR B 231		13.221	57.526	۷۵۰۶۵۷	1.00 32.04			•

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5	ATOM	9651	CG2	THR E	3 231	13.075	55.769	24.829		43.12			С
-	ATOM	9655	С		3 231	12.171	57.381	26.865	1.00	43.15			С
	ATOM	9656	0		3 231	13.088	57.379	27.628		49.59			0
	ATOM	9657	N	THR E		11.031	56.804	27.149	1.00	45.08			N
	ATOM	9659	CA	THR E		10.801	56.103	28.393	1.00	46.07			С
10		9661	СВ		3 232	9.344	55.581	28.375		43.69			С
10	MOTA			THR E		8.475	56.653	27.964		49.53			0
	MOTA	9663					55.276	29.748		43.76		•	C
	ATOM	9665		THR E		8.867				49.16			Č
	MOTA	9669	¢		3 232	11.759	54.905	28.630		51.59			ő
	ATOM	9670	0	THR E		12.563	54.922	29.567					N
15	MOTA	9671	N		3 233	11.660	53.899	27.757		51.81			
	ATOM	9673	CA		3 233	12.327	52.604	27.879		50.18			·C
	MOTA	9675	CB	ASN E	3 233	11.655	51.566	26.967		52.42			C
	ATOM	9678	CG	ASN E	3 233	10.276	51.148	27.383		52.34			С
	ATOM	9679	OD1	ASN I	3 233	9.680	51.677	28.321	1.00	50.82			0
20	ATOM	9680			3 233	9.750	50.153	26.650	100	52.61			N.
20	ATOM	.9683	C		3 233	13.729	52.350	27.416	1.00	47.14			С
		9684	Ö		B 233	14.259	52.963	26.555	1.00	46.63			0
	MOTA				B 234	14.306	51.355	28.019		47.70			N
	ATOM	9685	N			15.430	50.768	27.402		51.03			С
0.5	MOTA	9687	CA		B 234	15.430	49.591	28.256		47.48			Ċ
25	ATOM	9689	CB		B 234					44.91			Ċ
	ATOM		· CG		B 234	17.388	49.421	28.108	_				Ċ
	ATOM	9694			B 234	17.926	48.199	28.788		47.69			c
	ATOM	9698	CD2		B 234	17.643	49.365	26.676		49.15			
	ATOM	9702	С		B 234	14.716	50.251	26.142		53.66			C
30	ATOM	9703	0		B 234	13.639	49.694	26.270		57.67			0
	ATOM	9704	N	ARG :	B 235	15.262	50.431	24.945		54.47			N
	ATOM	9706	CA	ARG I	B 235	14.628	49.892	23.749		50.55		•	С
	ATOM	9708	CB	ARG :	B 235	14.146	50.948	22.782	1.00	54.70			. C
	ATOM	9711	CG		B 235	13.090	51.958	23.232	1.00	60.77			С
35 .	ATOM	9714	CD		В 235	11.610	51.498	23.022	1.00	63.38			C
.55.	ATOM	9717	NE		B 235	10.905	52.094	21.882	1.00	65.81			N
	ATOM	9719	CZ		B 235	10.487	51.422	20.806		68.02			C.
		9720			B 235	9.854	52.062	19.844		70.13			N
	ATOM	•			B 235	10.703	50.121	20.678		68.31			N
40	MOTA	9723				15.799	49.326	23.069		52.73			С
40	MOTA	9726	C		B 235		50.033	22.960		51.89			0
	MOTA	9727	0		B 235	16.794		22.591		53.67			N
	ATOM	9728	N		B 236	15.697	48.083	21.951		51.18			C
	MOTA	9730	CA		B 236	16.816	47.414						c
	MOTA	9732	CB		B 236	17.336	46.273	22.857		54.12			c
45	MOTA	9735	CG		236, B	17.606	46.565	24.346		54.84			
	ATOM	9737			B 236	17.445	45.294	25,170	-	59.47		٠ ^.	Ċ
	ATOM	9741	CD2	LEU	В 236	18.988				57.80			С
	MOTA	9745	С	PE A	B 236	16.472	46.882	20.555		49.66			С
	MOTA	9746	0	LEU	B 236	15.320	46.574	20.244	1.00	51.23			О
.50	ATOM	9747	N		B 237	17.516	46.802	19.740	1.00	49.55			N
. 4 0	ATOM	9748	CA		B 237	17.528	46.266	18.364	1.00	53.89		٠.	, C
	ATOM	9750	СВ		B 237	19.037	46.236	18.036	1.00	52.34			С
		9753	CG		B 237	19.634	47.291	18.888		51.34			С
	ATOM		CD		B 237	18.837	47.302	20.146		49.53	•		С
55	ATOM	9756			B 237		44.846	18.178		55.60			C
55	ATOM	9759	C			17.003		18.794		51.46			ō
	MOTA	9760	0		B 237	17.524	43.944					•	N
	MOTA	9761	N		B 238	16.027	44.660	17.297		62.69			
	MOTA	9763	CA		B 238	15.321	43.386	17.149		62.37			C
	MOTA	9765	CB		B 238	14.847	43.178	15.702		63.90			С
60	MOTA	9768	CG	LYS	B 238	14.017	41.850	15.476		67.48			C
	ATOM	9771	CD	LYS	B 238	12.652	41.826	16.191	1.0	70.44			С

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5	ATOM	9774	CE	LYS I	B 238	12.375	40.445	16.872	1.00 75.03	•	С
•	ATOM	9777.	NZ		3 238	10.906	40.068	17.069	1.00 74.40		N
	ATOM	9781			3 238	16.015	42.134	17.728	1.00 60.78		С
	ATOM	9782	ō		3 238	15.417	41.472	18.563	1.00 63.50		0
	ATOM	9783	N		3 239	17.242	41.808	17.318	1.00 62.12		N
10	ATOM	9785	CA		B 239	17.976	40.613	17.832	1.00 62.88		C
io		9787	CB		3 239 3 239	19.245	40.375	17.004	1.00 63.86		č
•	ATOM		•		B 239	19.081	39.310	15.932	1.00 71.17		č
	ATOM	9790	CG				39.144	15.035	1.00 73.03		Č
•	ATOM	9793	CD		B 239	20.316			1.00 74.08		c
16	ATOM	9796	CE		B 239	20.418	37.713	14.440	1.00 74.08		
15	ATOM	9799	NZ		B 239	20.797	37.688	12.972			N
	MOTA	9803	С		B 239	18.422	40.587	19.317	1.00 63.28		C
	ATOM	9804	Ο.		B 239	18.587	39.508	19.896	1.00 62.95		0
	MOTA	9805	N		B 240	18.627	41.760	19.915	1.00 58.01		, N
	MOTA	9807	CA		B 240	19.131	41.875	21.269	1.00 54.79	•	С
20	MOTA .	9809	CB	VAL 1	B 240	19.827	43.225	21.427	1.00 58.03		С
	ATOM	9811	CG1	VAL	B 240	20.256	43.484	22.875	1.00 57.45		С
	ATOM	9815	CG2	VAL 1	B 240	21.047	43.292	20.450	1.00 57.36		С
	ATOM	9819	C	VAL :	B 240	17.964	41.707	22.220	1.00 56.00		С
	ATOM	9820	0 .	VAL	B 240	17.980	40.890	23.143	1.00 52.22		0
25	MOTA	9821	N	PHE 1	B 241	16.928	42.488	22.012	1.00 55.23		. N
	ATOM	9823	CA		B 241	15.725	42.212	22.742	1.00 53.80		C
	ATOM	9825	СВ	PHE	B 241	14.545	42.796	22.032	1.00 51.30		С
	ATOM	9828	CG		B 241	13.300	42,770	22.822	1.00 47.65		С
	ATOM	9829			B 241	13.154	43.590	23.937	1.00 48.68		С
30	ATOM	9831			B 241	11.997	43.588	24.677	1.00 50.08		С
30	ATOM.	9833	CZ		B 241	10.952	42.755	24.315	1.00 51.83		· c
	ATOM	9835			B 241	11.085	41.930	23.193	1.00 54.34		С
	ATOM	9837			B 241	12.267	41.953	22.451	1.00 52.82		C
	ATOM	9839	C		B 241	15.546	40.714	22.793	1.00 55.05		Ċ
35	ATOM	9840	Ö		B 241	15.660	40.121	23.852	1.00 58.72		Ö
55	ATOM	9841	N		B 242	15.296	40.080	21.651	1.00 58.90		N
	ATOM	9843	CA		B 242	14.915	38.650	21.665	1.00 61.77		C
	ATOM	9845	CB		B 242	14.771	38.033	20.255	1.00 64.23		Ċ
	ATOM	9848	CG		B 242	13.434	38.214	19.518	1.00 66.72		C
40	ATOM	9851	CD		B 242	12.187	37.837	20.319	1.00 73.25		Č
70	ATOM .	9852			B 242	11.766	36.659	20.267	1.00 74.25		ō
		9853			B 242	11.605	38.724	20.207	1.00 80.65		ŏ
	MOTA				B 242	15.946	37.859	22.473	1.00 60.51		c
	ATOM	9854	C			15.606		23.317	1.00 61.16		ŏ
15	ATOM	9855	0		B 242		37.063				N
45	ATOM	9856	N		B 243	17.221	38.094	22.222	1.00 59.55		C
	ATOM	9858	CA		B 243	18.246	37.412	22.981	1.00 54.76 1.00 50.14	•	C
	ATOM	9860			B 243	19.628	37.910	22.546			
	MOTA	9864	С		B 243	18.056					C
-	ATOM	9865	0		B 243	18.157	36.691	25.272	1.00 60.16		0
50	MOTA	9866	N		B 244	17.764	38.868	24.872	1.00 60.67		N
	MOTA	9868	CA		B 244	17.847	39.252	26.277	1.00 56.99		С
	MOTA	9870	CB		B 244	17.983	40.721	26.396	1.00 54.73		С
	ATOM	9874	С.	ALA	B 244	16.670	38.756	27.039			, C
	MOTA	9875	0	ALA	B 244	16.814	38.027	28.022	1.00 66.61		0
55	ATOM	9876	· N	VAL	B 245	15.497	39.121	26.578	1.00 58.39		N
	ATOM	9878	CA	VAL	B 245	14.264	38.628	27.182	1.00 57.61		С
	ATOM	9880	CB	VAL	В 245	13.084	38.947	26.272	1.00 55.77		С
	ATOM	9882	CG1	VAL	B 245	11.921	38.046	26.582	1.00 60.16		С
	ATOM	9886	CG2	VAL	B 245	12.682	40.395	26.425	1.00 55.68		С
60	ATOM	9890	С		B 245	14.276	37.104	27.445	1.00 56.76		С
	MOTA	9891	0		B 245	13.735	36.630	28.457	1.00 58.98		0

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5	MOTA	9892	N	LYS B 246		14.863	36.289	26.581	1.00 54.47		N
	MOTA	9894	CA	LYS B 246		14.782	34.895	26.954	1.00 59.19		C
	MOTA	9896	CB	LYS B 246		15.091	33.852	25.848	1.00 58.81		C
	MOTA	9899	CG	LYS B 246		16.412	33.840	25.110	1.00 66.67		C
	ATOM	9902	ĊD	LYS B 246		16.771	32.349	24.732	1.00 73.69		C.
10	ATOM	9905	CE	LYS B 246		17.214	32.133	23.273	1.00 77.68	•	С
	MOTA	9908	NZ	LYS B 246		17.712	30.722	23.053	1.00 78.54		N
	MOTA .	9912	С	LYS B 246		15.610	34.750	28.221	1.00 60.14		C
٠.	ATOM	9913	0	LYS B 246		15.229	34.049	29.153	1.00 59.34		0
	ATOM	9914	N	SER B 247		16.715	35.484	28.265	1.00 59.55		N
15	ATOM	9916	CA	SER B 247		17.663	35.354	29.355	1.00 58.72		C
	ATOM	9918	CB	SER B 247		18.952	36.101	29.017	1.00 57.44		C
	ATOM	9921	OG	SER B 247		20.044	35.581	29.739	1.00 59.12		0
	MOTA	9923	С	SER B 247	•	17.082	35.830	30.676	1.00 58.15	٠.	C
	MOTA	9924	0	SER B 247		17.282	35.207	31.709	1.00 61.22		0
20	MOTA	9925	N	ILE B 248		16.339	36.915	30.632	1.00 55.00		N
	MOTA	9927	CA	ILE B 248		15.793	37.501	31.837	1.00 53.84		C.
	MOTA	9929		ILE B 248		15.123	38.845		1.00 53.06		C
	ATOM	9931		ILE B 248		16.196	39.788	30.939	1.00 51.58		C
	MOTA	9934		ILE B 248	•	15.656	41.103	30.457	1.00 55.81		C
25 .	ATOM	9938.	CG2	ILE B 248		14.381	39.461	32.661	1.00 52.52		C
	ATOM	9942	С	ILE B 248		14.821	36.536	32.460	1.00 54.27		· C
	MOTA	9943	0	ILE B 248		14.720	36.477	33.668	1.00 51.87		0
	ATOM	9944	N	LYS B 249		14.114	35.784	31.619	1.00 58.95	•	N
	MOTA	9946	CA	LYS B 249		13.080	34.863		1.00 63.35		C
30	MOTA	9948	CB	LYS B 249		12.386	34.163	30.895	1.00 67.38	•	C
	MOTA	9951	CG	LYS B 249		11.566	35.076	29.969	1.00 71.83	•	C
	MOTA	9954	CD	LYS B 249		10.893	34.193	28.921	1.00 72.34		C
	MOTA	9957	CE	LYS B 249		10.025	34.974	27.965	1.00 74.28		. N
	ATOM	9960	NZ	LYS B 249	·	10.188	34.448	26.585	1.00 75.13 1.00 64.05		C
35	ATOM	9964	С	LYS B 249		13.828	33.829	32.836	1.00 66.66		0
	ATOM	9965	0	LYS B 249		13.596	33.579	34.028 32.098	1.00 60.44		N
	ATOM	9966	N	ALA B 250		14.755 15.572	33.235 32.211	32.626	1.00 52.39		C
	ATOM	9968	CA	ALA B 250		16.787	32.061	31.812	1.00 32.35		č
40	ATOM	9970	CB C	ALA B 250 ALA B 250		15.897	32.687	33.993	1.00 53.08		Č
40	ATOM	9974 9975	0 -	ALA B 250		15.492	32.096	34.986	1.00 60.98		ō
	ATOM	9976	N	ALA B 251		16.602	33.792	34.071	1.00 55.04		N
	MOTA MOTA	9978	CA	ALA B 251		17.098	34.209	35.367	1.00 52.66		Ċ
	ATOM	9980	CB	ALA B 251		17.817	35.549	35,273	1.00 50.20		С
45	ATOM	9984	C	ALA B 251		15.943	34.276	36.333	1.00 52.91		· C
-15	ATOM	9985	ō	ALA B 251		16.084	33.908	37.476	1.00 63.90		0
	ATOM	9986	N	SER B 252		14.786	34.706	35.865	i.00 51.39		N
	ATOM	9988	CA	SER B 252		13.655			1.00 47.50		,C
	MOTA	9990	СВ	SER B 252		12.838	36.112	36.195	1.00 45.09		Ç
50	ATOM	9993	OG	SER B 252		12.937	36.176		1.00 44.57		Ó
•	ATOM	9995		SER B 252		12.744	33.741		1.00 46.38		С
	ATOM	9996	0	SER B 252		11.696	33.817	37.506	1.00 52.86		0
٠.	ATOM	9997	N	SER B 253		13.095	32.626	36.257	1.00 46.89		N
	ATOM	9999	CA	SER B 253		12.113	31.515	36.239	1.00 51.70		C
55	ATOM	10001	CB	SER B 253		12.694	30.258	35.673	1.00 49.29		С
	ATOM	10004	OG	SER B 253		12.622	29.350	36.744	1.00 50.36		0
	ATOM	10006	C	SER B 253		11.493	31.064	37.584	1.00 50.23		С
	ATOM	10007	0	SER B 253		10.549	30.335	37.570	1.00 48.06		0
	ATOM	10008	N	THR B 254		11.992	31.448	38.743	1.00 54.64		N
60	ATOM	10010	CA	THR B 254		11.303	30.979	39.944	1.00 55.86	•	С
-	MOTA	10012	CB	THR B 254		11.876	31.518	41.285	1.00 55.22		С
									• *		

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5	ATOM	10014		THR B			12.383	32.851	41.131		59.23			0
	ATOM	10016	CG2 '	THR E	254		13.081	30.702	41.690		57.98	•		C
	ATOM	10020	C '	THR E	254		9.853	31.304	39.850		56.31			Ċ
	ATOM	10021		THR E			9.067	30.740	40.587		58.63		•	0
	ATOM	10022		GLU E			9.496	32.222	38.954		63.22			N
10	ATOM	10024		GLU E			8.081	32.520	38.661	1.00	64.71			С
10		10024		GLU E			7.691	33.884	39.210	1.00	64.18			С
	ATOM	10029		GLU E			7.814	33.921	40.721	1.00	65.62			С
	ATOM				3 255		6.988	35.013	41.364	1.00	65.81			С
	MOTA	10032			3 255		5.941	35.412	40.801		65.88			O
	MOTA	10033					7.398	35.458	42.452		67.44			0
15	ATOM	10034			3 255		7.843	32.474	37.155		65.92			С
	MOTA	10035			3 255	•	8.761	32.231	36.374		67.96			0
	MOTA	10036			3 255			32.686	36.737		64.15	•		N
		10037			3 256		6.611	32.771			62.25			C
	MOTA	10039			3 256		6.347		35.319		65.89			Ċ
20	MOTA	10041			3 256		5.753	31.487	34.780		70.21			C
	MOTA	10044			B 256		6.795		34.631		71.31			Ċ
	MOTA	10047			B 256		7.580	30.472	33.304		70.80			Ċ
	ATOM	10050			B 256		8.688	29.418	33.197		70.80			N
	MOTA	10053	NZ		B 256	•	9.037	28.832	34.535					C
25	MOTA	10057	С		B 256		5.414	33.918	35.091		61.03			Ö
	ATOM	10058	0		В 256		4.620	34.277	35.977		57.24			N
	MOTA	10059	N		B 257		5.522	34.500	33.903		57.37			C
	ATOM	10061	CA	PHE :	В 257		4.700	35.632	33.563		58.14			C
	ATOM	10063	CB	PHE	B 257		5.557	36.904	33.635		57.69		•	
30	ATOM	10066	CG		В 257		6.262	37.095	34.971		52.26			C C
	ATOM	10067			В 257		7.620	36.875	35.098		55.74			C
	ATOM	10069	CEl		B 257		8.248	37.044	36.298		55.86			C
	MOTA	10071	CZ	PHE	B 257		7.530	37.444	37.391		56.14			
	ATOM	10073			B 257		6.194	37.666	37.274		54.82			C.
35 .	ATOM	10075	CD2	PHE	B 257		5.569	37.490	36.073		49.91			
	MOTA	10077	С	PHE	в 257		4.089	35.397	32.177		61.13			C
	MOTA	10078	. 0	PHE	В 257		4.687	34.705	31.356		60.35			0
	ATOM	10079	N	PRO	B 258		2.902	35.964	31.934		64.44			N
	ATOM	10080	CA		B 258		2.175	35.834	30.651		67.15			С
40	MOTA	10082	CB	PRO	B 258		0.765	36.286	31.018		65.96			C
	ATOM	10085	CG	PRO	В 258		0.946	37.246	.32.161		63.58			C
	ATOM	10088	CD	PRO	B 258		2.172	36.804	32.906		63.13			C
	ATOM	10091	С	PRO	B 258		2.740	36.758	29.561		71.79			С
	MOTA	10092	0	PRO	B 258		2.885	37.952	29.830		76.81			0
45	ATOM	10093	N	ASP	B 259		3.010	36.250			73.38			N
	ATOM	10095	CA	ASP	B 259	•	3.820	36.980	27.356		75.86			C
· .•	ATOM	10097	CB	ASP	B 259		3.890	36.221	26.029		0 77.62			C
	MOTA		CG	ASP	B 259		3.803				0 78.97			C
	MOTA				B 259		4.731	33.953	25.816		0 64.34			0
50	ATOM				B 259		2.814	34.178	26.786	1.0	0 80.20			0
50	ATOM		С		B 259		3.443	38.429	27.102		0 76.48			С
	ATOM		ō		B 259		4.216		26.500	1.0	0 74.95			0
	ATOM		N		B 260		2.259		27.548	1.0	0 75.19			N
	ATOM		CA		B 260		1.905		27.489	1.0	0 72.78			С
55			C.		B 260		2.926	_			0 68.86			С
در	ATOM		Ö		B 260		3.429				0.70.54			0
	ATOM	•	N		B 261		3.239				0 65.94			N.
	ATOM ATOM		CA		B 261		4.187				0 61.43			С
	ATOM				B 261		4.317	•			0 56.82			С
60					B 261		5.391				0 54.73			С
30	ATOM				B 261		5.126				0 51.57			'C
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                        LEU B 267
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            10231 C
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5	ATOM	10232	0	LEU I	3 267		0.742	42.633	34.643	1.00 65.04		О
	MOTA	10233	N	VAL 1	B 268	1	2.062	43.779	36.031	1.00 66.18		N
	ATOM	10235	CA	VAL I	B 268	'	2.201	42.665	36.966	1.00 63.11		С
	MOTA	10237		VAL I			3.526	42.035	36.844	1.00 63.47		C
	ATOM	10239	CG1	VAL 1	B 268	:	3.584	40.817	37.674	1.00 65.01		C.
10	MOTA	10243	CG2	VAL 1	B 268	;	3.741	41.689	35.434	1.00 67.71		
	MOTA	10247	С	VAL 1	B 268	}	2.089	43.146	38.376	1.00 62.57		С
	MOTA	10248	.0	VAL I	B 268	1	2.535	44.227	38.723	1.00 64.30		0
	ATOM	10249	N	CYS			1.498	42.320	39.204	1.00 62.51		N
	MOTA	10251	CA	CYS			1.189	42.742	40.543	1.00 62.84		C
15	ATOM	10253	CB	CYS	B 269		-0.334	42.937	40.667	1.00 64.89		C
	ATOM	10256	SG	CYS	B 269)	-0.978	44.253	39.612	1.00 68.14		S
	MOTA	10257	С	CYS			1.677	41.778	41.610	1.00 58.60		С
	MOTA	10258	0	CYS	B 269		1.707	40.556	41.420	1.00 57.72		0
•	ATOM	10259	N	TRP	B 270)	2.040	42.374	42.731	1.00 50.46		N
20	ATOM	10261	CA	TRP	B 270)	2.483	41.669	43.896	1.00 53.90		C
	MOTA	10263	CB	TRP	B 270)	3.996	41.833	44.087	1.00 54.89		С
	ATOM	10266	CG	TRP	B 27)	4.740	40.871	43.267	1.00 55.99		C
	ATOM	10267	CD1	TRP	B 27)	4.829	39.543	43.480	1.00 57.11		C.
	MOTA	10269	NE1	TRP	B 27)	5.601	38.961	42.503	1.00 61.98		N
25	ATOM	10271		TRP			6.026	39.929	41.633	1.00 61.92		С
	ATOM	10272		TRP			5.500	41.145	42.081	1.00 57.92		С
	MOTA	10273		TRP			5.793	42.297	41.355	1.00 53.37		С
	MOTA	10275	CZ3	TRP	B 27)	6.571	42.199	40.241	1.00 53.54		С
	ATOM	10277		TRP			7.083	40.982	39.812	1.00 56.68	•	C
30 ·	MOTA	10279	CZ2	TRP			6.825	39.834	40.490	1.00 64.93		C
	ATOM	10281	С		B 27		1.753	42.293	45.048	1.00 52.99		Ç
	ATOM	10282	0		B 27		1.321	43.432	44.976	1.00 52.30		0
	MOTA	10283	N		B 27		1.612	41.554	46.126	1.00 56.53		N
	MOTA	10285	CA		B 27		0.897	42.083	47.267	1.00 58.01 1.00 60.04		C
35	ATOM ·	10287	CB		B 27		0.936	41.079° 41.648	48.415 49.826	1.00 60.04		C
	ATOM	10290	CG		B 27		0.773	40.664	50.910	1.00 09.33		č
	ATOM	10293	CD		B 27		1.280 2.450	40.268	50.900	1.00 78.40		ŏ
	ATOM	10294		GLN			0.392	40.262	51.825	1.00 80.06	•	N
40	ATOM ATOM	10295 10298	C	GLN			1.683		47.553	1.00 54.15		C
40	ATOM	10299	0		B 27		2.781	43.454	47.050	1.00 62.98	•	0
	ATOM	10300	N ·		B 27		1.162	44.209		1.00 54.28		N
	ATOM	10300	CA		B 27		1.964	45.351	48.683	1.00 55.76		C
	ATOM	10302	CB		B 27		1.280	46.192	49.767	1.00 54.56		С
45	ATOM	10308			B 27		3.325	44.876	49.169	1.00 57.86		С
13	ATOM	10309		ALA			3.497	43.739	49.579	1.00 57.62		0
•	ATOM	10310	N		B 27		4.296	45.776	49.067	1.00 64.15		N
	ATOM	10312	CA		B 27			45.660	49.699	1.00 62.02		С
	ATOM	10315	С		B 27		6.435	44.431		1.00 59.47		C
50	ATOM	10316	0		B 27		7.544	44.376	50.003	1.00 62.91		0
	ATOM	10317	N		B 27		5.926	43.467	48.751	1.00 59.03		N
	ATOM	10319	CA		B 27		6.529	42.155	48.713	1.00 52.35		С
	ATOM	10321	СВ		В 27		5.483	41.091	49.087	1.00 58.59	•	С
	ATOM	10323					4.574	40.872	47.988	1.00 54.95		. 0
55	ATOM	10325		THR			4.593	41.579	50.243	1.00 55.11		С
	ATOM	10329			B 27		6.971	41.857	47.351	1.00 46.12		C.
	ATOM.	10330	0		B 27		6.961	40.726	46.957	1.00 46.68		О
	ATOM	10331	N		B 27		7.332	42.868	46.600	1.00 47.81		N
	ATOM	10333	CA		B 27		7.866			1.00 48.64		С
60	ATOM	10335	CB		B 27		8.257		44.540	1.00 47.68		С
	ATOM	10337	OG1	THR	B 27	5	7.090	44.596	44.064	1.00 50.08		0

										- 07			C	•
5	ATOM	10339	CG2	THR B 275		9.005	43.551	43.276	1.00 40	1 15			Ċ	
_	MOTA	10343	C	THR B 275		9.114	41.783	45.539	1.00 5	4 70		•	0	
	ATOM	10344	0	THR B 275		9.984	42.143	46.371					N	
	ATOM	10345	N	PRO B 276		9.190	40.685	44.822	1.00 4				Ċ	
	ATOM	10346	CA	PRO B 276		10.355	39.808	44.811	1.00 4				c	
10	ATOM .	10348	CB	PRO B 276		9.895	38.611	43.955	1.00 5				Ċ	
	ATOM	10351	CG	PRO B 276		8.574	38.955	43.383	1.00 5				Ċ	
	MOTA	10354	CD	PRO B 276		8.101	40.227	43.956	1.00 5	0.10				Š
	ATOM	10357	С	PRO B 276		11.557	40.420	44.091	1.00 4					
	ATOM	10358	0	PRO B 276		12.010	39.796	43.088	1.00 4))
15	ATOM	10359	N ·	TRP B 277		12.083	41.567	44.537	1.00 4					N
13	ATOM	10361	CA	TRP B 277		13.120	42.230	43.711	1.00 4					C
	ATOM	10363	CB	TRP B 277		13.740	43.469	44.393	1.00 4					C .
	ATOM	10366	CG	TRP B 277		12.769	44.677	44.518	1.00 5					C
	ATOM	10367		TRP B 277		12.309	45.236	45.680	1.00 5					С
20		10369		TRP B 277		11.463	46.285	45.412	1.00 4					N
20	MOTA	10303		TRP B 277		11.359	46.429	44.063	1.00 4					С
	ATOM	10371	CD2	TRP B 277		12.164	45.439	43.466	1.00 4					С
	MOTA			TRP B 277		12.222	45.390	42.078	1.00 5					C,
	MOTA	10373		TRP B 277		11.486		41.352	1.00 4	6.11				С
0.5	MOTA	10375		TRP B 277		10.703	47.270	41.991	1.00 4	5.63				С
25	ATOM	10377		TRP B 277		10.626		43.337	1.00 4	2.71				С
	MOTA	10379		TRP B 277		14.202	41.229	43.271	1.00 4					С
	MOTA	10381	C .	TRP B 277		14.664	41.180	42.123	1.00 4					0
•	ATOM	10382	0			14.594	40.388	44.184	1.00 5					N
	ATOM	10383	N	ASN B 278		15.742	39.549	43.918	1.00		•			С
30	ATOM	10385	CA	ASN B 278		16.264	39.003	45.227	1.00					С
	ATOM	10387	CB	ASN B 278		15.300	38.046	45.876	1.00					C
	MOTA	10390	CG	ASN B 278	٠	15.630	36.887	46.122	1.00					0
	MOTA	10391		ASN B 278			38.528	46.162						N
	MOTA	10392		2 ASN B 278		14.095	38.410	42.941	1.00		•			С
35	ATOM	10395	С	ASN B 278	•	15.579	37.810	42.616	1.00				•	0
	MOTA	10396	0	ASN B 278		16.577	38.074	42.447	1.00					N
	ATOM	10397	N	ILE B 279		14.384	36.960	41.496	1.00					С
	MOTA	10399	CA	ILE B 279		14.356	36.227	41.370	1.00					С
	MOTA	10401	CB	ILE B 279		13.006	37.181	41.143	1.00					C
40	MOTA	10403		1 ILE B 279		11.844		40.444	1.00					С
	MOTA	10406	CD.	1 ILE B 279		10.671	36.467	42.562	1.00			٠.		C.
	MOTA	10410	CG:	2 ILE B 279		12.724	35.335	42.302		47.23				C
	MOTA	10414	С	ILE B 279		14.796		39.311		48.85				o
	ATOM	10415	0	ILE B 279		15.121		39.886		51.85				N
45	MOTA	10416	N	PHE B 280		14.809				43.99				C
	ATOM	10418	CA			15.181	39.313			47.60				c
	MOTA					14.346				50.69				C
	ATOM	10423	CG	PHE B 280		12.840								C
	ATOM		CD	1 PHE B 280		12.157				47.59				.C
50	MOTA			1 PHE B 280		10.793				49.69				C
-	ATOM		CZ	PHE B 280		10.114				53.43			•	C
	ATÓM			2 PHE B 280		10.792				50.88				
٠	ATOM		CD	2 PHE B. 280	•	12.126	40.407			44.76				C
	ATOM	•		PHE B 280		16.604				43.94				C
55	ATOM			PHE B 280		17.114	40.282			43.28				0
رر	ATOM			PRO B 281		17.256				37.73				N
	ATOM		CA	. PRO B 281		18.668		37.413		33.44				C
	ATOM			001		19.089				36.50				C
		_				18.034			1.00	38.20				С
<i>د</i> ٥	MOTA						39.358		1.00	39.79			,	С
60	MOTA	·		PRO B 281		18.928				36.85				, C
	ATOM	1 10448	, ,	***** P POT										

_	2 0014	10410	_	DDO 1	201	10 020	41 004	26 527	1 00 42 07		^
5 .	ATOM	10449	0		B 281	18.039	41.984	36.537	1.00 43.97		0
	MOTA	10450	N		B 282	20.144	41.806	37.290	1.00 42.26		N
•	ATOM	10452	CA		B 282 .	20.585	43.141	36.983	1.00 39.23		C
	ATOM	10454	CB		B 282	21.818	43.477	37.809	1.00 43.53		С
	MOTA	10456			B 282	21.497	43.457	39.275	1.00 40.33		С
10	ATOM	10460	CG2	VAL 1	B 282	22.988	42.465	37.444	1.00 39.80		С
	ATOM	10464	С	VAL 1	B 282 -	21.100	43.067	35.569	1.00 41.69		С
	ATOM	10465	0	VAL	B 282	21.582	42.011	35.184	1.00 35.21	•	0
	ATOM	10466	N	ILE !	B 283	21.025	44.169	34.819	1.00 39.90		N
•	MOTA	10468	CA	ILE I	В 283	21.558	44.219	33.457	1.00 39.37		. С
15	MOTA	10470	СВ		B 283 .	20.505	44.748	32.505	1.00 40.29		C
	ATOM	10472			B · 283	19.273	43.855	32.531	1.00 35.95		С
	ATOM	10475			B 283	18.066	44.572	32.090	1.00 41.11		С
	ATOM	10479			B 283	21.074	44.867	31.102	1.00 33.71		С
	ATOM	10483	C		B 283	22.709	45.198	33.425	1.00 46.04	:	c
20	ATOM	10484	o		B 283	22.691	46.233	34.110	1.00 49.32		0
20	ATOM	10485	N		B 284	23.709	44.885	32.612	1.00 48.26	•	N
	ATOM	10487	CA		B 284	24.893	45.713	32.522	1.00 46.53		C
	ATOM	10489	CB		B 284	26.088	44.939	33.112	1.00 44.99		č
	ATOM	10492	OG		B 284	25.927	44.696	34.522	1.00 44.94		ŏ
25	ATOM	10494	C		B 284	25.206	46.048	31.086	1.00 46.23		, č
23	ATOM	10494			B 284	25.284	45.130	30.269	1.00 51.09		. 0
	ATOM	10495	O N		B 285	25.388	47.325	30.764	1.00 41.48		, N
	ATOM	10498	CA		B 285	25.877	47.669	29.447	1.00 39.92		C
	ATOM .	10490	CB		B 285	24.939	48.679	28.756	1.00 35.47		Č
30	ATOM	10503	CG		B 285	23.394	48.570	28.921	1.00 38.05		Č
50						22.708	49.787	28.300	1.00 35.50		č
:	ATOM	10505 10509			B 285 B 285	22.708	47.308	28.356	1.00 33.30		Ċ
	ATOM	10503	C		B 285	27.330	48.156	29.671	1.00 37.32		č
	ATOM	10513			B 285	27.562		30.617	1.00 37.44		Ö
35	ATOM ATOM	10514	O N		B 286	28.288	47.684	28.850	1.00 37.44		. N
33	MOTA	10517	CA		B 286	29.697	48.167		1.00 45.00	•	C
	ATOM	10517	CB		B 286	30.698	47.012	28.685	1.00 46.18		č
	ATOM	10522	CG		B 286	30.744	45.888	29.752	1.00 48.12		č
	ATOM	10523			B 286	29.678	45.025	29.975	1.00 47.49		č
40.	ATOM	10525			B 286	29.767	44.036	30.934	1.00 46.99	•	č
1.0	ATOM	10523	CZ		B 286	30.945	43.911	31.667	1.00 49.87		. Č
	ATOM	10528	OH		B 286	31.134	42.952	32.643	1.00 45.54		Ö
	ATOM	10530			B 286	31.986	44.753	31.444	1.00 45.24		č
	ATOM	10530			B 286	31.892	45.699	30.511	1.00 43.24	-	C
45	ATOM	10532	CDZ		B 286	29.917	49.065	27.602	1.00 46.95	•	C
43 .	ATOM	10535	Ö		B 286	29.613	48.633	26.494	1.00 43.90		ő
•	ATOM	10536	N		B 287	30.480	50.269	27.782	1.00 42.38		N
	ATOM	10538	CA		B 287	30.526	51.257	26.741	1.00 40.41		Ċ
	ATOM	10530	CB		B 287	29.874	52.562	27.203	1.00 40.41		c
50							52.664			•	c
υŅ	MOTA	10543	CG		B 287	28.487 28.344		27.896	1.00 35.23		C
	ATOM	10545			B 287 B 287	27.480	53.994	28.625	1.00 37.04		C
	ATOM ATOM	10549			B 287	31.960	52.558	26.938	1.00 26.22		C
•		10553					51.571	26.564	1.00 45.87		
55	ATOM	10554	0		B 287	32.716	51.400	27.474	1.00 51.50		0
55	ATOM	10555	N			32.356	52.041 52.315	25.401	1.00 50.25		N
	MOTA	10557	CA		B 288	33.749		25.123	1.00 52.89		C
	MOTA	10559 10562	CB		B 288	33.884	52.619	23.654	1.00 57.49		C
	MOTA	10565	CG SD		B 288 _. B 288	35.255 35.108	52.585 53.029	23.075 21.308	1.00 59.46 1.00 62.39		C
		10707	511		n /xx	33.108	22.074	7.1.308	1 DU 62 40		S
60	ATOM										
60	ATOM ATOM	10566 10570	CE.	MET	B 288 B 288	35.316 34.157	51.616 53.518	20.631 25.927	1.00 56.14 1.00 55.91		. C

											- 04			0	
5	ATOM	10571		MET B			33.354	54.433	26.109	1.00				N	
J			N	GLY B	289		35.403	53.522	26.405	1.00				C	
	• • • • • •		CA	GLY E	289		35.911	54.608	27.230	1.00				C	
	ATOM		С	GLY E	3 289		36.880	55.482	26.473	1.00				0	
	ATOM			GLY E			37.113	55.267	25.286	1.00					
10	ATOM	10579	N		3 290.		37.460	56.465	27.143	1.00				С И	
10	ATOM	10581	CA	GLU F			38.341	57.390	26.444	1.00				c	
	ATOM	10583	СВ	GLU E			38.373	58.726	27.150	1.00					
	ATOM	10586	CG		3 290		37.021	59.394	27.100	1.00				. C	
	ATOM	10589	CD.		3 290		37.125	60.824	26.612	1.00					
15	ATOM	10590	OE1	GLU I	3 290	•	37.333	61.687	27.500	1.00				0	
15		10591	OE2	GLU I	B 290		37.006	61.078	25.360	1.00				0	
	ATOM		·C	GLU I	B 290		39.767	56.919	26.220		61.97			C	
	ATOM	10592	0		В 290		40.377	57.319	25.243	1.00	65.39			0	
•	MOTA	10594	N		B 291		40.325	56.086	27.090	1.00	62.97			N	
20	ATOM	10596	CA		B 291		41.697	55.643	26.854		61.83			. C	
20	MOTA		CB		B 291		42.336	55.119	28.158		63.23			C.	
	MOTA	10598			B 291		43.820	54.897	27.988	1.00	67.30			С	
-1.	MOTA	10600			B 291		42.121	56.153	29.281		66.27		•	С	
	ATOM:	10604	C		B 291		41.452	54.644	25.731		59.22			C.	
05	ATOM	10608			B 291		40.303	54.325	25.463	1.00	56.93			0	
25	MOTA	10609	0		B 292		42.468	54.169	25.038		58.29			N	
	MOTA	10610	N		B 292		42.227	53.183	23.969		59.67			С	
	MOTA	10612	CA		B 292		43.311	53.327	22.909	1.00	62.91			C	
	MOTA	10614	CB		B 292		42.746	53.895	21.712	1.00	63.26			0	
	MOTA	10616	0G1		B 292		43.859	51.953		1.00	62.53			С	
30	MOTA	10618	CG2		B 292		42.280	51.766	24.494	1.00	57.76			С	
	ATOM	10622	C		B 292		43.004	51.517	25.393	1.00	57.85			0	
	MOTA	10623	0		B 292		41.535	50.819	23.968		61.18			N	
	ATOM	10624	N		B 293		41.737	49.429	24.428		66.82			С	
~ -	MOTA	10626	CA		B 293		43.237	49.258	24.806	i.00	.71.42			С	
. 35	MOTA	10628	CB		B 293		44.001	48.005	24.291	1.00	73.25	٠.	•	С	
•	MOTA	10631	CG		В 293		45.538	48.253	24.118	1.00	76.24			С	
٠.	MOTA	10634	CD		B 293		46.178	47.731	23.180	1.00	73.24			. 0	
	MOTA	10635	OET	CIN	B 293		46.111	49.048	25.015	1.00	73.09			И	
40	MOTA	10636			B 293		40.883			1.00	66.33			С	
40	ATOM	10639	C		B 293		40.602		_	1.00	69.45			. 0	
	ATOM	10640	0		B 293		40.467				64.46			N	
	ATOM	10641	N		B 294		39.810			1.00	57.83			С	
	MOTA	10643	CA	CIN	B 294		40.597				58.59			C	
4.5	ATOM		CB		В 294		40.167				57.32			C	
45	ATOM		CG		В 294		41.418				62.05			С	
	MOTA		CD		B 294		41.355			1.00	72.12.			0	
	MOTA						42.570				60.53	•		И	
•	ATOM			2 GPN	B 294		38.287				57.84			С	
	MOTA				B 294	. <i>.</i>	37.830				56.18			. 0	
50	ATOM				B 294						54.23			N	
	ATOM				В 295		37.490				53.45			Ċ	
	ATOM				В 295		36.050				52.98			, C	
•	ATOM				В 295		35.178				0 55.81			0	
	ATOM				В 295		35.006				0 49.98			C	
55	ATOM				В 295		35.503				0 47.16			ō	
	· ATOM		0		В 295		36.119				0 47.10			N	
	ATOM				В 296		34.34				0 46.25			C	
	ATON	1 10671			В 296		33.70				0 45.49			Ċ	
	ATON				В 296		33.85				0 43.49			Ċ	
60			ce.		E B 296		32.90				0 47.00			. 0	
	ATON		CI	O1 PHE	В 296		31.72	3 52.55	0 32.13	J 1.0	J 47.00				

	•						•								
5	MOTA	10679	CE1	PHE B	296	:	30.808	53.551	32.396		39.26				C
-	ATOM	10681	CZ	PHE B	296	:	31.089	54.394	31.341		40.65				C .
	MOTA	10683	CE2	PHE B	296	:	32.268	54.266	30.638		37.93				С
	ATOM.	10685	CD2	PHE B	296		33.159	53.302	30.984		39.04				С
	ATOM	10687	C.	PHE B	296	. :	32.232	49.871	31.423	1.00	48.20				С
10	ATOM	10688	0	PHE B		;	31.778	49.499	30.341		54.42				0
10	ATOM	10689	N ·	ARG B			31.501	49.849	32.544	1.00	45.88				N
	MOTA	10691	CA	ARG B			30.130	49.426	32.526	1.00	43.75				С
	ATOM.	10693		ARG B		:	30.058	47.928	32.696		46.61				С
	ATOM	10696	CG	ARG B			30.812	47.407	33.875	1.00	52.65				С
15	ATOM	10699	CD	ARG B			30.556	45.919	34,138	1.00	52.49				C
1,5	MOTA	10702	NE		297		30.710	45.525	35.546	1.00	51.81				N
	ATOM	10704	CZ	ARG E			31.212	44.358	35.939	1.00	48.75				· C
	ATOM	10705		ARG E			31.614	43.487	35.042	1.00	53.62				N
. •	ATOM	10708		ARG E			31.317		37.222	1.00	43.21				N
20	ATOM.	10711	C	ARG E			29.314	50.074	33.615	1.00	47.03		•		С
.20	ATOM	10712	ō	ARG E			29.852	50.469	34.676	1.00	48.02				0
•	ATOM	10713	N	ILE E			28.010	50.187	33.294	1.00	45.30				N
	ATOM.	10715	CA	ILE E			26.937	50.674	34.150	1.00	44.58				C
	ATOM	10717	CB		3 298		26.152	51.846	33.497	1.00	42.21				С
25	ATOM	10719		ILE E				51.391	32.217		40.03				С
23	ATOM	10713		ILE E			24.548	52.508	31.592		39.09				С
	ATOM	10726		ILE E			27.077	52.977	33.228		43.78				С
	ATOM	10720	C		3 298		25.987	49.471	34.284	1.00	45.83	:			С
	MOTA	10731	Ö		3 298		25.735	48.749	33.325	1.00	38.32				0
30	ATOM	10731	N		B 299		25.443	49.270	35.467		46.26				N
.50	MOTA	10732	CA		B 299		24.696	48.072	35.721		47.54				C ·
	ATOM	10734	CB	THR I			25.575	47.181	36,607		52.72				С
	ATOM	10738		THR I			26.587	46.537	35.810		52.36				0
	ATOM	10740		THR			24.789	46.025	37.227		53.54				С
35 -	ATOM	10744	C		B 299		23.441	48.459	36.439		47.53				С
بدد	ATOM	10745	Ö		B 299		23.554	49.107	37.478	1.00	45.39		•		0
	. ATOM	10746	N		В 300 .		22.265	48.087	35.887	1.00	47.99				N
	ATOM	10748	CA.		В 300		20.952	48.367	36.518		46.84				С
	ATOM	10750	CB		в 300		19.924	49.104	35.627	1.00	46.77				С
40	MOTA	10752			в 300		19.842	48.506	34.244	1.00	45.61				C .
-10	ATOM	10755			в 300		18.475	48.734	33.633	1.00	46.44				С
	ATOM	10759			в 300		20.194	50.538	35.586	1.00	52.09				С
	ATOM	10763	C		B 300	•	20.186	47.167	36.971	1.00	44.73				Ç
	ATOM	10764	ō		в 300		20.413	46.046	36.543	1.00	43.89				0
45	ATOM	10765	N		в 301		19.231	47.509	37.816	1.00	46.21				N
	ATOM	10767	CA.		в 301		18.355	46.631	38.524	1.00	44.01			•	C
•	ATOM	10769	CB		в 301		18.303	47.094	39.973	1.00	47.01		•		С
•	ATOM	10772	CG	LEU	В 301		19.419	47.990	40.471	1.00	40.39				С
	ATOM	10774			в 301		19.093	48.496	41.828	1.00	40.91				С
50	ATOM	10778			в 301		20.671	47.123	40.543	1.00	47.03				С
50 .	ATOM	10782	·C		в 301		16.936	46.740	38.060	1.00	46.44				С
	ATOM	10783	ō		В 301		16.540	47.644	37.336	1.00	43.22				0
	ATOM	10784	N		В 302		16.136	45.819	38.547		51.74				N
	ATOM	10785	CA		В 302		14.748	45.738	38.120		47.89				C
55 ·	ATOM	10787	CB		В 302		14.282	44.417	38.721	1.00	51.94	•			С
55	MOTA	10790	.CG		B 302		15.105	44.241	39.916		53.36				С
	ATOM	10793	CD		B 302		16.475	44.793	39.553		53.46				С
	ATOM	10796	С		B 302		14.008	46.884	38.695		43.06				C
	ATOM	10797	ō		B 302		12.940	47.149			42.92	•			0
60	ATOM		N		В 303		14.582	47.561	39.681		42.87				N
00			CA	CI.N	в 303		13.930	48.707	40.253		42.11				С
	MOTA	10000	CH	GTI14	÷ 505		. 10.550		,						

								504	1 00 40 42			C ·
5	ATOM	10802	CB	GLN B 303		14.625	49.192	41.504	1.00 40.42			
	MOTA	10805	CG	GLN B 303		14.037	48.667	42.758	1.00 40.53			C
	ATOM	10808	CD	GLN B 303		14.744	47.461	43.285	1.00 43.06			C
	MOTA	10809		GLN B 303		15.546	46.827	42.579	1.00 39.84			0
	ATOM	10810		GLN B 303		14.449	47.126	44.543	1.00 43.69			N
10		10813	C	GLN B 303		14.061	49.794	39.271	1.00 45.98			C,
10	MOTA			GLN B 303		13.689	50.934	39.528	1.00 53.51			0
	MOTA	10814				14.602	49.469	38.129	1.00.47.03			N
	MOTA	10815	N	GLN B 304		14.815	50.478	37.174	1.00 46.42			C.
	MOTA	10817	CA	GLN B 304				36.921	1.00 48.97			С
	MOTA	10819	CB	GLN B 304		16.294	50.534		1.00 45.42			C
15	MOTA.	10822	CG	GLN B 304		16.894	51.900	37.204	1.00 43.42			Ċ
	MOTA	10825	CD	GLN B 304.		17.282	52.050	38.613				Ö
	MOTA	10826		GLN B 304		16.869	52.990	39.271	1.00 55.93		·	N
	MOTA	1.0827	NE2	GLN B 304		18.088	51.152	39.088	1.00 43.68			
•	ATOM	10830	С	GLN B 304		14.081	50:144	35.904	1.00 51.85			С
20	MOTA	10831	0	GLN B 304		13.344	51.021	35.361	1.00 53.64			0
20	ATOM	10832	N	TYR B 305		14.276	48.905	35.420	1.00 49.13			N
	ATOM	10834	CA	TYR B 305		13.624	48.452	34.192	1.00 48.73			С
		10836	CB	TYR B 305		14.445	47.418	33.409	1.00 48.24			С
	MOTA		CG	TYR B 305	•	14.696	46.120	34.075	1.00 45.68			С
25	ATOM	10839				13.829	45.057	33.906	1.00 49.08			С
25	ATOM	10840		TYR B 305		14.056	43.872	34.505	1.00 51.64			С
		10842		TYR B 305			43.711	35.301	1.00 59.15			С
	ATOM ·		CZ	TYR B 305		15.186			1.00 61.84			. 0
	MOTA	10845	OH	TYR B 305		15.454	42.500	35.932	1.00 56.26		·	Ċ
	MOTA	10847		TYR B 305		16.063	44.765	35.467				Ċ.
. 30	MOTA	10849	CD2	TYR B 305		15.805	45.948	34.857	1.00 48.39			c
	ATOM	10851	С	TYR B 305		12.264	47.897	34.416	1.00 51.41			
	MOTA	10852	0	TYR B 305		11.637	47.411	33.467	1.00 50.10			0
	MOTA	10853	N	LEU B 306		11.807	47.952	35.662	1.00 51.83			И
	ATOM	10855	CA	LEU B 306		10.481	47.474	35.996	1.00 49.68			C
35	ATOM	10857	CB	LEU B 306		10.508	46.481	37.129	1.00 52.01			C
<i>J</i> .	ATOM	10860	CG	LEU B 306		10.687	45.019	36.827	1.00 51.56			С
	ATOM	10862		LEU B 306		10.108	44.267	38.015	1.00 53.34			С
	MOTA	10866		LEU B 306		9.924	44.708	35.605	1.00 56.13			С
		10870	C	LEU B 306		9.884	48.717	36.499	1.00 50.94			С
40	ATOM		ŏ	LEU B 306		10.282	49.209	37.547	1.00 50.28			0
. 40	MOTA	10871		ARG B 307		8.908	49.212	35.764	1.00 49.70			N
	ATOM	10872	N			8.419	50.538	35.974	1.00 44.12			C
	ATOM	10874	CA	ARG B 307		8.456	51.259	34.633	1.00 38.83			С
	MOTA	10876	CB	ARG B 307	• .		52.549	34.573	1.00 42.47			С
	MOTA	10879	CG	ARG B 307		7.667			1.00 46.67			C
45	MOTA	10882	CD	ARG B 307		7.695	53.176	33.188	1.00 49.09			N
	ATOM	.10885	NE	ARG B 307		6.899	52.434	32.208				C
	. ATOM	10887	CZ	ARG B 307	•	5.744	52.870		1.00 55.81			N
•	ATOM	10888	NH1	L ARG B 307		5.245	54.035	32.116				
	MOTA	10891	NH2	2 ARG B 307		5.072	52.145					N
50	ATOM		С	ARG B 307		7.038	50.495	36.548				С
20	ATOM	•	Ó	ARG B 307		6.218	49.805	35.992	1.00 51.23	L		0
	ATOM			PRO B 308		6.799	51.239	37.629	1.00 46.48	3.		N
		*		PRO B 308		5.547				•		С
	MOTA			PRO B 308		5.892						С
~ ~	MOTA					7.261			1.00 49.0			С
55	MOTA			PRO B 308		7.773				3		С
	MOTA			PRO B 308								C
	ATOM			PRO B 308		4.465						Ō
	ATOM			PRO B 308		4.792						N
	MOTA			VAL B 309		3.200						c
60	ATOM					2.026						c
	ATOM	10914	CB	VAL·B 309)	1.720	51.597	35.938	1.00 65.0	U		C

		1									•
5	ATOM	10916	CGl	VAL	В	309	2.994	51.101	35.294	1.00 63.7	8 C
	ATOM	10920	CG2	VAL	В	309	0.825	50.415	36.150	1.00 64.8	
	ATOM	10924	С	VAL	B	309	0.810	52.137	38.173	1.00 64.3	
	ATOM	10925	0	VAL	В	309	0.764	51.261	39.002	1.00 55.4	3 0
	ATOM	10926	N	GLU			-0.215	52.936	37.977	1.00 70.9	2 N
10	ATOM		CA	GLU			-1.368	52.762	38.834	1.00 74.9	
10	ATOM	10930	СВ	GLU			-2.380	53.877	38.651	1.00 76.8	
	ATOM	10933	CG	GLU			-3.286	54.103	39.862	1.00 82.9	
٠.	ATOM	10936	CD			310	-2.610	53.829	41.205	1.00 84:0	
	ATOM	10937		GLU			-2.619	52.653	41.631	1.00 90.2	
15	ATOM	10938		GLU			-2.082	54.774	41.841	1.00 83.2	
10	ATOM	10939	С	GLU			-1.978	51.443	38.473	1.00 76.1	
	ATOM	10940		GLU			-1.908	51.029	37.296	1.00 76.2	
	ATOM	10941	N	ASP			-2.558	50.766	39.470	1.00 78.5	
٠.	ATOM	10943	CA	ASP			-3.306	49.539	39.182	1.00 82.1	
20	ATOM!	10945	СВ	ASP			-3.558	48.684	40.441	1.00 82.6	
	ATOM	10948		ASP			-3.918	47.211	40.111	1.00 83.4	
	ATOM	10949		ASP			-4.210	46.905	38.926	1.00 86.0	
	ATOM	10950		ASP			-3.931	46.295	40.976	1.00 76.7	
	ATOM	10951	C	ASP			-4.643	49.948	38.570	1.00 83.7	•
25	ATOM	10952	ō	ASP			-5.174	51.026	38.867	1.00 81.5	
23	ATOM	10953	N	VAL			-5.172	49.100	37.707	1.00 85.5	
	ATOM	10955	CA	VAL			-6.496	49.341	37.181	1.00 88.9	
	ATOM	10957	СВ	VAL			-7.065	48.064	36.499	1.00 88.3	•
	ATOM.	10959		VAL			-8.222	48.405	35.595	1.00 88.2	
30	ATOM	10963		VAL			-5.979	47.356	35.697	1.00 88.5	
50	ATOM	10967	C	VAL			-7.361	49.769	38.383	1.00 92.5	
	ATOM	10968	o	VAL			-7.811	50.910	38.482	1.00 94.9	•
• (ATOM	10969		ALA			-7.563	48.866	39.331	1.00 96.0	
	ATOM	10971	CA			313	-8.432	49.151	40.470	1.00 97.3	
35	ATOM	10973	CB	ALA			-8.438		41.424	1.00 95.5	
55	ATOM	10977	C	ALA			-8.055	50.404	41.281	1.00 98.1	
	ATOM	10978	ō	ALA			-8.868	50.852	42.088	1.00102.3	
	ATOM	10979	N	THR			-6.864	50.971	41.033	1.00 97.4	
	ATOM	10981	CA	THR			-6.102	51.818	42.013	1.00 96.5	
40	ATOM	10983	CB	THR			-6.505	53.356	42.037	1.00 95.7	
	ATOM	10985		THR			-7.547	53.635	42.985	1.00 95.9	
•	ATOM	10987					-7.040	53.811	40.662	1.00 95.1	
:	ATOM	10991	С	THR			-6.028	51.095	43.417	1.00 94.9	
	ATOM	10992	o ·			314	-6.148	51.703	44.505	1.00 89.2	
45	ATOM	10993		SER			-5.810	49.767	43.307	1.00 94.7	
		10995	CA	SER			-5.731	48.796	44.424	1.00 93.4	
	ATOM	10997	ĊB	SER			-5.712	47.335	43.911	1.00 93.2	
	ATOM		OG	SER			-4.568	47.043		1.00 85.8	
	ATOM	11002	C	SER			-4.516	49.033		1.00 93.2	
50	ATOM	11003	Ō	SER			-3.681	49.893	44.995	1.00 94.1	
	ATOM	11004	N	GLN			-4.410	48.279	46.404	1.00 91.5	
	ATOM	11006		GLN			-3.318	48.533	47.354	1.00 91.2	
·	ATOM	11008	CB	GLN			-3.756	48.294	48.839	1.00 92.3	
•	ATOM	11011	CG	GLN			-4.329	49.622	49.500	1.00 93.0	
55	ATOM	11014	CD	GLN			-4.619	49.576	51.022	1.00 91.3	
	ATOM	11015		GLN			-4.691	48.505	51.626	1.00 90.8	
	ATOM	11016	NE2	GLN			-4.791	50.762	51.629	1.00 89.3	
	ATOM	11019	c	GLN			-2.010	47.823	46.923	1.00 85.4	
	ATOM :		ō	GLN			-0.926	48.158		1.00 84.7	
60	ATOM	11021	N	ASP			-2.129	46.872	46.001	1.00 78.1	
	ATOM	11023	CA	ASP			-0.980	46.180	45.434	1.00 76.1	
					_	,		10,100		10.1	_

· 5	ATOM	11025	CB	ASP	В	317		-1.492	45.121	44.472	1.00 73.46	5		С
	ATOM	11028	CG	ASP	В	317		-2.262	44.078	45.184	1.00 72.17	,		С
	MOTA	11029	OD1	ASP	В	317		-2.407	44.252	46.424	1.00 70.34	<u> </u>		0
	MOTA	11030	OD2	ASP	В	317		-2.743	43.073	44.620	1.00 70.32	2		0
	ATOM	11031	С	ASP	В	317		0.034	47.099	44.728	1.00 76.88	3		С
10	ATOM	11032	0	ASP	В	317		-0.247	48.268	44.447	1.00 82.57	,		0
	ATOM	11033	N	ASP	В	318		1.216	46.558	44.448	1.00 74.00)		N
	ATOM	11035	CA	ASP	В	318		2.304	47.312	43.838	1.00 68.80	, .		C
	MOTA	11037	ÇВ	ASP	В	318		3.577	47.191	44.686	1.00 70.82	2		C
	ATOM	11040	CG	ASP	В	318		3.534	48.035	45.962	1.00 71.07	,		С
15	ATOM	11041	OD1	ASP	В	318		4.185	47.662	46.968	1.00 70.80)		0
	ATOM	11042	OD2	ASP	В	318		2.884	49.087	46.052	1.00 73.30)		0
	ATOM	11043	- · C	ASP	В	318		2.511	46.719	42.455	1.00 65.62	:		. С
	MOTA	11044	0	ASP	В	318		3.019	45.608	42.319	1.00 60.87	· .		0
	ATOM	11045	N	CYS	В	319		2.126	47.456	41.419	1.00 61.57)		N
20	ATOM	11047	CA	CYS	В	319	•	2.133	46.872	40.093	1.00 57.97	,	•	С
	ATOM	11049	CB	CYS	В	319		0.736	46.962	39.463	1.00 61.08	;		С
	ATOM	11052	SG			319		-0.613	46.137	40.403	1.00 68.12	!	•	S
	ATOM	11053	С	CYS	В	319		3.220	47.524	39.269	1.00 52.64			С
	ATOM	11054	0			319		3.745	48.540	39.662	1.00 52.88			0
25	ATOM	11055	N	TYR	В	320		3.560	46.945	38.130	1.00 47.04			N
	MOTA	11057	CA	TYR	В	320		4.728	.47.385		1.00 50.79)		C
	ATOM	11059	CB	TYR	В	320		6.042	46.773	38.010	1.00 51.87	_		C
	ATOM	11062	CG	TYR	В	320		6.341	47.116	39.469	1.00 44.28			С
	ATOM	11063	CD1	TYR	В	320		5.861	46.331	40.512	1.00 51.75	i		C
30	ATOM	11065	CE1	TYR	В	320		6.125	46.637	41.826	1.00 48.81			С
	ATOM	11067	CZ	TYR	В	320		6.873	47.737	42.090	1.00 51.67			С
•	ATOM	11068	OH	TYR	В	320		7.161	48.090	43.379	1.00 63.11			. 0
	ATOM	11070	CE2	TYR	В	320		7.351	48.512	41.073	1.00 46.32			C
	ATOM	11072	CD2	TYR	В	320		7.082	48.188	39.779	1.00 35.82			С
35	· ATOM	11074	С	TYR	В	320		4.626	46.882	36.016	1.00 52.12			С
	ATOM	11075	0	TYR	В	320		4.082	45.809	35.792	1.00 56.07			0
	MOTA	11076	N	LYS	В	321		5.164	47.667	35.085	1.00 53.09			N
	ATOM	11078	CA	LYS	В	321		5.216	47.294	33.708	1.00.51.68			С
	MOTA	11080	CB	LYS	В	321		4.684	48.430	32.832	1.00 57.10)		С
40 .	ATOM	11083	CG	LYS	В	321		3.102	48.538	32.635	1.00 61.86	5		С
	ATOM	11086	CD	LYS	В	321		2.727	49.287	31.269	1.00 67.16	;		С
	MOTA	11089	CE	LYS	В	321		1.532	50.345	31.323	1.00 70.93	3		С
	MOTA	11092	NZ	LYS	В	321		1.847	51.846	31.459	1.00 71.64			N
	MOTA	11096	С	LYS	В	321		6.681	47.049	33.421	1.00 49.27	•		С
45	ATOM	11097	0	LYS	В	321		7.544	47.694	33.987	1.00 54.13	3.		0
	ATOM		· N	PHE	В	322		6.961	46.083	32.568	1.00 45.37	' <i>.</i> .		N
•	MOTA	11100	CA	PHE				8.291	45.825		1.00 45.16			С
	MOTA	11102	CB	PHE				8.218	44.478	31.390	1.00 41.79)		C.
	MOTA	11105	CG	PHE	В	322		9.528	43.929	30.875	1.00 42.80	1	٠.	C
50	MOTA	11106		PHE				10.627	43.747	31.697	1.00 41.54			C
	MOTA	11108	CE1	PHE	В	322		11.812	43.202	31.188	1.00 46.06	; <u>,</u>		C
•	ATOM	11110	CZ	PHE	В	322		11.895	42.839	29.861	1.00 44.89)	-	С
	MOTA	11112		PHE				10.803	43.031	29.042	1.00 34.54			C
	ATOM	11114	CD2	PHE	В	322		9.633	43,.549	29.547	1.00 37.25	,		С
55	ATOM	11116	C	PHE	В	322		8.606	46.957	31.087	1.00 48.75	,		С
	ATOM	11117	Ο.	PHE	В	322		7.894	47.126	30.099	1.00 56.32			0
	MOTA	11118	N	ALA				9.651	47.736	31.346	1.00 49.68			N
	MOTA	11120	CA	ALA				10.098	48.768	30.413	1.00 46.88			C
	MOTA	11122	CB	ALA				10.314	50.060	31.172	1.00 46.63			С
60	MOTA	11126	C	ALA				11.377	48.461	29.609	1.00 45.38			С
	MOTA	11127	0	ALA		323		12.397	49.107	29.792	1.00 55.92			0
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     MOTA
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                     PHE B 345
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                                             64.181
     MOTA
           11443
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                  CD2. PHE B 345
     MOTA
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                     PHE B 345
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     MOTA
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                                     32.313
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                  OD2 ASP B 346
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                                     29.506
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                                                     26.081
                      ARG B 347
     ATOM
           11461 N
                                     29.637
                                             68.935
                                                     24.701
                                                            1.00 43.73
     ATOM 11463
                      ARG B 347
                  CA
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								co oco	24.423	1 00	43.30			С
5	ATOM	11465	CB	ARG I	В 347		28.570	69.962			42.11			c
_	MOTA	11468	CG	ARG !	B 347		27.202	69.356	24.324					c
•	ATOM	11471	CD	ARG !	В 347		26.079	70.326	24.660		46.02			
	ATOM	11474	NE		в 347		25.906	71.409	23.697		46.95			N
		11476	CZ		В 347		25.579	71.248	22.418		49.44			С
10	MOTA				В 347		25.401	70.035	21.910	1.00	48.15			N
10	MOTA	11477	NUT	ARG .	D 247		25.433	72.313	21.632	1.00	51.53			Ñ
	MOTA	11480			B 347		30.988	69.558	24.396		48.71			C.
	MOTA	11483	С		B 347			69.455	23.286		49.46			0
	ATOM .	11484	0		В 347		31.492		25.379		49.23			N
	MOTA	11485	N		B 348		31.578	70.217			46.88			C
15	MOTA	11487	CA		B 348		32.842	70.875	25.172					Ċ
	ATOM	11489	CB	ALA	B 348		33.226	71.682	26.425		48.10			Č.
	ATOM	11493	С	ALA	B 348		33.901	69.837	24.849		53.46			
	ATOM	11494		ALA	B 348		34.834	70.103	24.076		54.08			0
•	ATOM	11495	N		B 349		33.768	68.641	25.426		54.97			N
20					B 349		34.773	67.599	25.178		51.50			С
20	MOTA	11497			В 349		35.395	67.153	26.517	1.00	50.57			С
	MOTA	11499	CB				36.426	68.192	27.060		50.96			С
	ATOM	11502	CG		B 349		36.963	67.948	28.466		53.35			С
	MOTA	11505	CD		B 349			66.891	28.506		58.63			N
	MOTA	11508	NE		В 349		37.988		29.599		60.78			C
25	MOTA	11510	\mathbf{CZ}		В 349		38.667	66.554			54.92			N
	ATOM	11511	NH1	ARG	в 349		38.427	67.189	30.747					N
	ATOM	11514	NH2	ARG	B 349		39.585	65.593	29.545		61.55		:	C.
	ATOM	11517	C:	ARG	B 349		34.290	66.413	24.305		50.33			
٠.	ATOM	11518	0		B 349		34.994	65.398	24.150		50.96	• .		0
30	MOTA	11519	N		в 350		33.103	66.532	23.724		46.02			N
30		11521	CA		В 350		32.610	65.465	22.881		46.35			С
	ATOM		CB		В 350		33.496	65.367	21.601	1.00	49.69			С
	ATOM	11523			B 350		33.014	64.434	20.402	1.00	58.03			С
	MOTA	11526	CG				33.785	64.714	19.003		58.14			, C
	MOTA	11529	CD		B 350		33.765		17.760					C.
35 .	ATOM	11532	CE		B 350					1 00	56.11			N
	ATOM	11535	NZ		в 350		33.683		23.717		.44.86			C.
	MOTA	11539	С		B 350		32.554				48.76			0
	MOTA	11540	O.		в 350		32.810				44.60			N
	MOTA	11541	N		B 351		32.200							C
40	ATOM	11543	CA	ARG	В 351		32.015) 44.48			c
• •	MOTA	11545	CB	ARG	В 351		33.225				43.82			c
	ATOM	11548	CG	ARG	В 351		33.540	64.024			45.18			
	ATOM	11551	CD		В 351		34.789	63.898	28.392		0 40.95			С
		11554	NE		В 351		34.687	64.715	29.598		0 46.55			N
15	MOTA				B 351		35.630		30.519	1.0	0 43.31			С
45	MOTA	11556			B 351		36.756				0 41.89			N
	ATOM	11557					35.456				0 54.20			N
	· ATOM				B 351	•	30.791				0 41.64			С
	MOTA				B 351						0 50.18			. 0
	ATOM	11564	0		B 351		30.368				0 38.69			Ņ
50	ATOM	. 11565			Е В 352		30.257				0 45.01	•		C
	ATOM		· CA		В 352	• .	29.130							c
	MOTA		CE	ILF	Е В 352		28.098				0 49.66			
	ATOM				Е В 352		27.315				0 52.66			. C
	ATOM				Е В 352		26.048	3 60.70€	26.013		0 56.74			C
55					E B 352		27.127		28.506		0 52.33			С
23	ATOM				E B 352		29.550			1.0	0 46.49		•	C
	ATOM				E B 352		30.129				0 45.55			0
	ATOM						29.23			1.0	0 46.26			N
	ATOM				Y B 353						0 44.22			. C
	MOTA				Y B 353		29.63				0 40.63			С
60	ATOM				Y B 353		28.530				0 50.25			Ō
	ATOM	1 11590	0	GL.	Y B 353		27.45	4 60.643	1 32.343	, 1.0	,, ,,,,,,			•

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5	MOTA	11591	N	PHE B 354		28.815	58.960	33.096	1.00 41.57				N
٠,	ATOM	11593	CA	PHE B 354		27.860	58.254	33.937	1.00 35.69				С
	ATOM	11595	СВ	PHE B 354		27.614	56.866	33.365	1.00 42.54				С
		11598	CG	PHE B 354		27.032	56.890	31.992	1.00 48.12				С
•	ATOM			PHE B 354		27.843	57.064	30.896	1.00 47.79				С
	ATOM	11599		PHE B 354		27.311	57.107	29.652	1.00 53.15				С
10	ATOM	11601				25.957	56.971	29.486	1.00 51.31				С
	MOTA	11603	CZ	PHE B 354			56.790	30.572	1.00 45.30			•	С
	ATOM	11605		PHE B 354		25.146	56.757	31.809	1.00 42.69				C
٠	MOTA	11607		PHE B 354		25.670		35.324	1.00 37.73				C
	ATOM	11609	С	PHE B 354		28.418	58.065	35.479	1.00 36.56				0
15	MOTA	11610	0	PHE B 354		29.561	57.648		1.00 34.99				N
	ATOM	11611	N	ALA B 355		27.611	58.364	36.333					c
	ATOM	11613	CA	ALA B 355		27.973	58.081	37.695	1.00 31.85	•			C
	ATOM	11615	CB	ALA B 355		28.631	59.305	38.285	1.00 35.10				
-	ATOM	11619	C	ALA B 355		.26.740	57:630	38:531	1.00 34.75				C
20	ATOM	11620	O	ALA B 355		25.641	58.105	38.363	1.00 38.79				.0
20	ATOM	11621	N	VAL B 356		26.909	56.686	39.430	1.00 36.60	•			N
		11623	CA	VAL B 356		25.801	56.261	40.272	1.00 35.07				C.
	MOTA	11625	CB	VAL B 356		26.370	55.348	41.344	1.00 32.99				C
	ATOM			VAL B 356		25.358	55.012	42.383	1.00 38.64		•		C
	ATOM	11627				26.829	54.112	40.710	1.00 35.78				\mathbf{c}
25	MOTA	11631	CG2			25.077	57.477	40.879	1.00 35.09				С
	MOTA	11635	C	VAL B 356			58.401	41.338	1.00 40.54				0
	MOTA	11636	0	VAL B 356		25.717		40.905	1.00 41.74				N
	ATOM	11637	N	SER B 357		23.752	57.483		1.00 41.57				C
	MOTA	11639	CA	SER B 357	•	22.999	58.670	41.346	1.00 47.83				Č
30	ATOM	11641	CB.			21.721	58.803	40.523					ŏ
	ATOM	11644	OG	SER B 357		21.001	60.008	40.844	1.00 50.14				Č
	ATOM	11646	С	SER B 357		22.591	58.706	42.805	1.00 44.92				Ö
	MOTA	11647	0	SER B 357		22.032	57.767	43.335	1.00 49.30				N
	MOTA	11648	N	ALA B 358		22.822	59.824	43.458	1.00 47.90				
35	ATOM	11650	CA	ALA B 358	٠	22.455	59.955	44.856	1.00 50.90				C
	ATOM	11652	CB	ALA B 358		22.871	61.301	45.346	1.00 52.95				C
	ATOM	11656	С	ALA B 358		20.962	59.764	45.155	1.00 51.41				C,
	ATOM	11657	0.	ALA B 358		20.538	59.955	46.293	1.00 50.45				0
	MOTA	11658	N	CYS B 359		20.158	59.408	44.167	1.00 51.99				N
40	ATOM	11660	CA	CYS B 359		18.739	59.237	44.444	1.00 56.13				.C
40	ATOM	11662	CB	CYS B 359		17.928	60.518	44.118	1.00 57.03				C
	ATOM:		SG	CYS B 359		17.612	60.710	42.327	1.00 70.47				S
	ATOM	11666	C	CYS B 359		18.122		43.726	1.00 51.20				С
				CYS B 359		16.907	58.001	43.614	1.00 57.81				0
16	ATOM			HIS B 360		18.909	57.107	43.238	1.00 46.00				N
45	ATOM	11668	N			18.286		42.602	1.00 46.33	}			С
		11670				19.256		41.736	1.00 43.36				С
		11672	CB			20.215			1.00 38.68				С
	MOTA		.CG	HIS B 360				42.996					N
	MOTA			1 HIS B 360		21.398		43.613					C
50	ATOM	11678	CE	1 HIS B 360		22.052	53.864						N
	ATOM	11680	NE	2 HIS B 360		21.334							c
	ATOM	11682	CD	2 HIS B 360		20.178							c
	MOTA			HIS B 360		17.608							
	ATOM			HIS B 360		18.049							0
55	ATOM			VAL B 361		16.521							N
	ATOM					15.712	53.536						C
	ATOM			1 0.54	•	14.359							Ċ
	ATOM) CC	1 VAL B 361		13.659			1.00 50.2	7			С
				2 VAL B 361		13.474			1.00 49.2	2			С
60	ATOM			VAL B 361		16.427				6			С
UU	ATOM			VAL B 361		16.805							. 0
	ATOM	1 11701	L O	AWD D 20T		20.000							

5	ATOM	11702	N	HIS B 362	16.636	51.656	45.235	1.00 50.40	•	N
		11704		HIS B 362	17.322	50.373		1.00 54.92		С
		11706		HIS B 362	18.864	50.539	45.254	1.00 54.49		C
	ATOM	11709		HIS B 362	19.377	51.443	46.321	1.00 60.33		С
	ATOM	11710		HIS B 362	19.017	52.771	46.390	1.00 66.26		N
10	ATOM >			HIS B 362	19.596	53.328	47.442	1.00 65.09		С
Ļ	ATOM	11714		HIS B 362	20.305	52.406	48.065	1.00 61.43		N
	ATOM	11716		HIS B 362	20.174	51.216	47.389	1.00 61.57		С
	ATOM			HIS B 362	16.929	49.742	46.671	1.00 54.45		С
	ATOM	11719		HIS B 362	16.069	50.242	47.362	1.00 53.82	٠.	0
15	ATOM	11720		ASP B 363	17.564	48.650	47.059	1.00 53.43		N
15		11722		ASP B 363	17.217	48.054	48.320	1.00 54.67		С
	MOTA	11724		ASP B 363	16.494	46.752	48.043	1.00 56.65		С
	MOTA	11727		ASP B 363	17.334	45.830	47.255	1.00 56.00		C.
-	MOTA	11728		ASP B 363	18.346	45.373	47.833	1.00 60.63		0
20	MOTA			ASP B 363	17.083	45.532	46.063	1.00 51.94		0
20		11729		ASP B 363	18.443	47.756	49.171	1.00 55.74	',	С
	ATOM	11730	С	ASP B 363	19.562	48.178	48.890	1.00 54:34		0
	ATOM-	11731	0	GLU B 364	18.180	46.998	50.216	1.00 54.75		N
	MOTA	11732	N		19.153	46.627	51.197	1.00 58.19		С
غہ	ATOM	11734	CA	GLU B 364	18.486	45.696	52.252	1.00 66.95	,	С
25	ATOM	11736	CB	GLU B 364	17.379	44.737	51.746	1.00 73.62		C
	ATOM	11739	CG	GLU B 364		45.284	51.760	1.00 79.77		C
	MOTA	11742		GLU B 364	15.939	46.193	50.945	1.00 81.19		Ō
	MOTA	11743		GLU B 364	15.620	44.780	52.581	1.00 79.52		0
	ATOM	11744		GLU B 364	15.110		50.655	1.00 53.23	•	C
30	ATOM	11745	С	GLU B 364	20.436	46.015	51.142	1.00 62.76		ō
	MOTA	11746		GLU B 364	21.497	46.365 45.146	49.652	1.00 48.86		N
	MOTA	11747	N	PHE B 365	20.359	-	49.032	1.00 45.25		C
	MOTA	11749	CA	PHE B 365	21.509	44.351	49.213	1.00 47.71		C
	ATOM	11751	CB	PHE B 365	21.180	42.866	50.568	1.00 47.71		č
35	MOTA	11754	CG	РНЕ В 365	20.355		50.470	1.00 47.10		Ċ
	ATOM	11755		PHE B 365	19.002	42.462	51.573	1.00 50.48	•	č
	ATOM	11757		PHE B 365	18.227	42.134	52.769	1.00 50.39		,C
	ATOM	11759	CZ	PHE B 365	18.807	41.860		1.00 30.35		Ċ
	MOTA	11761		PHE B 365	20.163	41.906	52.892 51.784	1.00 43.23		Ċ
40	MOTA	11763		PHE B 365	20.941	42.236		1.00 32.37		C C
	MOTA	11765	С	PHE B 365	22.028	44.401	47.758	1.00 48.65		ō
	MOTA	11766	0	PHE B 365	22.790	43.488	47.355 46.959	1.00 40.03		N
	MOTA	11767	Ν.	ARG B 366	21.628	45.387		1.00 38.21		c
	MOTA	11769	CA	ARG B 366	22.110		45.595	1.00 38.21	•	č
45	ATOM	11771		ARG B 366	21.196		44.631	100 45.53		č
•	MOTA .	··· 11774	CG	ARG B 366	21.366	•	44.547		-	č
	MOTA	11777	CD	ARG B 366	21.069		43.182	1.00 47.33		N
	MOTA	11780	NE	ARG B 366	19.640		42.943	1.00 46.43		· C
•	MOTA	11782	CZ	ARG B 366	18.989		42.253	1.00 48.01		. N
50	ATOM	· 11783	NH1	ARG B 366	19.682		41.765			N
	ATOM	11786	NH2	2 ARG B 366	17.671		42.048			C
	MOTA	11789	С	ARG B 366	21.978		45.262		•	
	ATOM	11790	0	ARG B 366	21.091		45.778			0
	ATOM	11791	N	THR B 367	22.812		44.353			N
55	ATOM	11793	CA	THR B 367	22.890					,C
	ATOM	. 11795	CB	THR B 367	23.905		45.030	1.00 48.16		C
	ATOM			THR B 367	23.712		45.171			0
	ATOM			2 THR B 367	25.310	49.228	44.422			C
	ATOM			THR B 367	23.342	49.094				C
60	ATOM			THR B 367	24.218	48.423	42.196			0
, 50	ATOM			ALA B 368		50.097	42.088	1.00 49.08		N
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OE1 GLU B 371 31.380 47.199
OE2 GLU B 371 30.602 46.566
C GLU B 371 33.499 50.071
O GLU B 371 32.935 49.921
N GLY B 372 34.842 50.169
CA GLY B 372 35.850 49.814
C GLY B 372 37.272 49.955
O GLY B 372 37.433 50.174
N PRO B 373 38.339 49.869
CA PRO B 373 38.339 49.869
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35.572
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                         THR B 376
     ATOM 11917
                     CB
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5	ATOM	11919	OG1	THR B	376		36.993	46.575	26.932	1.00 8	8.06			0
,	ATOM	11921	CG2	THR B	376		35.986	44.970	25.508	1.00 8	6.58			С
	MOTA	11925		THR B			39.130	45.590	24.246	1.00 9	0.80			С
	ATOM	11926		THR B			39.889	46.565	24.111	1.00 9	3.52			0
		11927		LEU B			38.840	44,768	23.240	1.00 9	4.98			N
10	ATOM			LEU B			39.572	44.884	21.974	1.00 9	7.54			С
10	MOTA	11929		LEU B			40.491	43.667	21.839	1.00 9	7.95			С
	ATOM	11931	CB	LEU B			41.234	43.239	23.119	1.00 9				С
	MOTA	11934	CG				42.302	42.213	22.767	1.00 9	6.01			C
	MOTA	11936		LEU B			41.873	44.413	23.852	1.00 9				С
	MOTA	11940		LEU B	3//			45.053	20.662	1.00 9	8.30			С
15	MOTA	11944	C	LEU B			38.777		20.470	1.00 9	5.52			o
	MOTA	11945	Ο.	LEU. B			37.719	44.425	19.782	1.00 9				N
	MOTA	11946	N	ASP E	378		39.328	45.909	18.405	1.00 9				C
	MOTA	11948	CA	ASP E			38.846	46.107	17.631	1.0010				c
	MOTA	11950	CB	ASP E			38.818	44.778		1.0010				Ċ
20	MOTA	11953	CG	ASP E			40.161	44.040	17.668	1.0010		*		ŏ
	ATOM	11954		ASP E			40.185	42.823	17.348	1.0010				Ö
	ATOM	11955	OD2	ASP E			41.238	44.594	18.001					č
	ATOM	11956	С	ASP E			37.466	46.678	18.517	1.00 9				Ö
	MOTA	11957	0	ASP E			36.576	46.473	17.690	1.00				N
25	MOTA	11958	N	MET I	3 379	٠	37.315		19.584	1.00				C
	ATOM	11960	CA		3 379		36.018	47.850	19.970	1.00 8			•	c
	ATOM	11962	CB	MET I	3 379		36.115	48.778	21.181	1.00 8				
	ATOM	11965	CG	MET I	3.79		36.814	48.131	22.363	1.00 8				C
	ATOM	11968	SD	MET I	3 379	•	36.294	48.757	23.944	1.00				S
30	ATOM	11969	CE	MET I	3 3 7 9		37.408	49.948	24.177	1.00				С
50	ATOM	11973	C·		в 379		35.455	48.535		1.00				C
	ATOM	11974	0		в 379		34.453	48.097	18.241	1.00				0
	ATOM	11975	N		в 380		36.133	49.590	18.349	1.00				N
	ATOM	11977	CA		B 380		35.555	50.483	17.361	1.00				C
35		11979	СВ		B 380		36.642	51.168	16.508	1.00				C
<i>33</i> .	ATOM	11982	CG		B 380		36.336	52.614	16.072	1.00				C
	ATOM	11985	CD		в 380		34.854	52.999	16.089	1.00				С
	ATOM	11986		GLU	В 380		34.530	54.085	16.634		82.43			0
	ATOM	11987			в 380		34.021	52.227	15.552	1.00				0
40	ATOM	11988	C		B 380		34.529	49.668	16.547		90.22			C
	MOTA	11989	. 0		в 380		33.385	50.102	16.385		89.91			0
	ATOM	11990.			B 381		34.946	48.482	16.080		89.23			N
	ATOM	11992	CA		B 381		34.122	47.536	15.284	1.00	85.33			С
	ATOM	11994			B 381		34.705	46.142	15.374	1.00	86.39			С
45	MOTA	11997	CG		B 381		35.859	45.959	14.456	1.00	91.21	•		С
. 33	MOTA	11998			B 381		35,821		13.353		93.25			0
	MOTA	11999	· OD2	ASP	B 381		36.842		14.742	1.00	97.75			0
	ATOM				B 381		32.676		15.606	1.00	79.23	•		С
		12001	ő		B 381		31.926				79.04			0
50	MOTA	12002			B 382		32.270				73.79			N
50	MOTA		CA		B 382		30.891				72.63			С
	ATOM	•			B 382		30.801	47.291	18.685		73.33			С
	MOTA						32.081				72.63			S
	ATOM				B 382		30.101				70.89			С
	ATOM				B 382		28,891		16.388		71.67	•		0
55	ATOM				B 382		30.838				72.45			N
	ATOM				B 383		30.295				71.23			С
	ATOM				B 383		29.732				69.89			C
	ATOM				B 383		30.294				73.05	•		0
حمر	ATOM				B 383		28.597			•	67.13			N
60	ATOM				B 384		27.915				64.11			C
	ATOM	12021	CA	TYR	в 384		21.31.	, 50.450	, ,,,,,,,,					

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	5	ATOM	12023	CB.	TYR B	384		26.468	50.421	13.020	1.00 61.05		C	
	_	ATOM	12026		TYR B			25.620	50.091	11.867	1.00 59.89		С	
		ATOM	12027		TYR B			25.280	48.777	11.578	1.00 59.47		С	
		ATOM	12029		TYR B			24.476	48.469	10.515	1.00 61.28		С	
	•	ATOM	12031		TYR E			23.997	49.497	9.733	1.00 62.97		С	
	10		12032		TYR E			23.179	49.288	8.636	1.00 63.75		0	
	10	ATOM			TYR E			24.332	50.792	10.028	1.00 64.64		С	
	•	MOTA	12034					25.136	51.079	11.083	1.00 60.10		С	
		ATOM	12036		TYR E			28.185	51.536	11.732	1.00 68.06		С	
		ATOM	12038		TYR E			28.365	52.708	12.106	1.00 67.06		0	
		MOTA	12039		TYR E				51.178	10.464	1.00 71.13		N	
	15	ATOM	12040		ASN E			28.213		9.438	1.00 74.74		C	
		MOTA	12042		ASN E			28.501	52.166	8.828	1.00 76.30		Č	
		MOTA	12044		ASN E			29.894	51.890		1.00 78.44		č	
	-	MOTA	12047		ASN I			31.057	51.931	9.889	1.00 76.44		Ö	
		ATOM	12048		ASN I			30.989	52.640	10.887			N	
	20	MOTA	12049	ND2	ASN I			32.111	51.163	9.646	1.00 76.88		C	•
		ATOM	12052	С	ASN I	3 385		27.362	52.205	8.374	1.00 79.12		Ö	
		MOTA	12053	0		385 .		27.234	51.384	7.455	1.00 79.49			
		MOTA	12054	TXO	ASN I	385 B		26.445	53.064	8.344	1.00 79.4		. 0	•
		ATOM	12055	N	SER (C -2		53.798	42.195	56.398	1.00 54.33		N	
	25	ATOM	12057	CA	SER C	C -2		54.991	42.203	57.314	1.00 54.20		С	
		ATOM	12059	CB	SER (C -2		54.496	42.894	58.620	1.00 59.83	Ļ	С	
		ATOM	12062	OG	SER (C -2		53.217	43.571	58.434	1.00 50.0		0	
		ATOM	12064	С	SER (55.846	40.853	57.607	1.00 51.30)	С	
		ATOM	12065	0	SER			56.969	40.946	58.008	1.00 52.4	1	0	
	30	ATOM	12068	N	PHE			55.366	39.626	57.416	1.00 49.5)	N	
	50	ATOM	12070	CA	PHE			56.183	38.439	57.772	1.00 45.0	3	С	
		ATOM	12072	СВ	PHE			55.401	37.604	58.777	1.00 45.1)	С	
		ATOM	12075	CG	PHE			54.686	38.446	59.773	1.00 43.7	4	С	
		ATOM	12076		PHE			53.717	39.362	59.347	1.00 39.8	1	С	
	35	ATOM	12078		PHE			53.068	40.151	60.248	1.00 44.6	2	C	
	22	ATOM	12080	CZ	PHE			53.371	40.058	61.605	1.00 39.3	9	C	
٠		ATOM	12082		PHE			54.336	39.149	62.031	1.00 45.6	0 ·	C	
		ATOM	12084		PHE			54.990	38.355	61.111	1.00 39.7	7	С	
		ATOM	12086	C	PHE			56.784	37.524	56.676	1.00 47.5	9	C	
	40	ATOM	12087	. 0	PHE			56.404	36.379	56.469	1.00 48.7	3 .	0	
	40	ATOM	12088	N	VAL			57.769	38.075	56.011	1.00 46.8	2	N	
		ATOM	12090	CA	VAL			58.543	37.462	54.968	1.00 42.5	6	C	
	-	ATOM	12092	СВ	VAL		•	59.695	38.359	54.783	1.00 48.9	9	Ċ	;
	•	ATOM	12094		VAL			59.357	39.397	53.764	1.00 51.1	0	C	;
	45	ATOM	12098		VAL			60.001	39.049	56.107	1.00 51.8		C	;
	73	MOTA	12102	C	VAL			59.140	36.107	55.089	1.00 46.0	4	C	;
		ATOM	12102	Ö	VAL		•	59.300	35.444	54.090	1.00 52.4	8		
	•		12104	N	GLU			59.520	35.666	56.275	1.00 52.4	0		1
		ATOM	12104	CA	GLU		•	60.053	34.310	56.418	1.00 48.0		C	
	50	MOTA	12108	CB	GLU			60.580		57.864	1.00 52.2		(
	50	ATOM			GLU			61.892	33.262	57.999			. (3
		ATOM	12111	CG				61.893					C	
		ATOM		CD	GLU			61.939					(
		ATOM	12115		GLU			61.884	30.928					c
	E C	ATOM			GLU			58.883						2
	55	ATOM			GLU									5
		ATOM			GLU			59.026						N
		ATOM			MET			57.696						C
	•	ATOM			MET			56.532						C
	~	MOTA			MET			55.626					ì	C
	60	MOTA			MET			56.231	33.224					S
		MOTA	12129	SD	MET	C 2		55.044	33.016	. 00.320	1.00 31	,,,	•	_

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	ATOM	12474	ō	GLN (25			61.039	16.151	61.274		46.44				0
10	ATOM	12475	N	THR		26			62.595	16.092	59.643	1.00	49.81				N
10	ATOM	12477	CA	THR		26			61.754	16.827	58.751	1.00	51.29				С
			CB	THR		26			62.462	17.098	57.429		53.77				С
	MOTA	12479		THR		26			63.759	17.659	57.673		53.98				Ó
•	MOTA	12481				26			61.709	18.172	56.629		52.68				С
	MOTA	12483 -		THR					60.555	15.969	58.478		51.30				С
15	MOTA	12487	С	THR		26				14.771	58.226		51.90				0
	ATOM	12488	0 ,	THR		26		٠.	60.666		58.530		50.70				N
	ATOM	12489	N	LEU		27	٠.	÷	59.396	16.594			43.30				C
	MOTA	12491	CA	LEU		27			58.174	15.933	58.155						Č
	MOTA	12493	CB	LEU		27		•	57.478	15.409	59.378		44.64				C
20	MOTA	12496	CG	TEO		27			58.218	14.449	60.281		45.47	•			C
	ATOM	12498		LEU		27	٠.		57.624	14.540	61.675		45.75				
	ATOM	12502	CD2	LEU	С	27			58.122	13.034	59.686		44.30				C
	ATOM	12506	. C	LEU	С	27			57.323	17.006	57.577		39.69				C
	ATOM	12507	0	LEU	С	27			57.495	18.143	57.925		43.38				0
.25	ATOM	12508	N	ASN		28			56.412	16.652	56.695		42.74				N
20	ATOM	12510	CA	ASN		28			55.433	17.586	56.185	1.00	41.37				С
	ATOM	12512	CB	ASN		28			55.194	17.347	54.703	1.00	42.25				. C
	ATOM	12515	CG	ASN		28			56.215	18.014	53.828	1.00	41.51				С
	ATOM	12516		ASN		28			56.417	17.614	52.679	1.00	48.06				0
20		12517		ASN		28			56.870	19.034	54.355		48.36				N
30	ATOM			ASN		28			54.144	17.326	56.948		42.07			•	С
	ATOM	12520	C	ASN		28			53.796	16.175	57.196		42.00				0
	ATOM	12521	0			29		٠	53.429	18.388			41.25				N
	MOTA	12522	N	ILE					52.254	18.282	58.144		38.11				С
25	ATOM	12524	CA	ILE		29	٠.			18.909	59.452		37.30				С
35 .	ATOM	12526	CB	ILE		29			52.581 53.888	18.345	60.002		37.82				C
	ATOM	12528		·ILE		29				16.947	60.383		37.89				Ċ
	MOTA	12531	CDI	ILE	C	29	•		53.764		60.382		37.26				Č
	ATOM	12535		ILE		29			51.428	18.758	57.605		41.88		•		Ċ
	ATOM	12539	Ç	ILE		29			51.111	19.100			44.35	-			ō
40	MOTA	12540	0	ILE		29			51.317	20.272	57.471		41.50				N
*.	MOTA	12541	N	LEU		30			49.924	18.485			40.03	٠.			.C
	ATOM	12543	CA	LEU		30			48.669	19.159	57.062			. •			C
	MOTA	12545	СВ	TEU		30			47.609	18.121	56.699		36.38				č
	MOTA	12548	. CG	PEA		30	٠.		46.175	18.515	56.462		43.90				c
45	MOTA	12550		LEU		30			45.650	17.851	55.272		48.94				·C
• • •	MOTA	12554	CD2	LEU		30			45.293	18.120	57.618		49.66				c
	ATOM	12558	С	LEU		.30			48.071	20.130	58.085	•	41.43				
	MOTA	12559	0	LEU	С	30			47.961				44.99				0
	MOTA	12560	N	VAL	С	31		٠	47.656	21.300	57.607		44.35				N
50 .	MOTA	12562	CA	VAL	C	31			47.080	22.312	58.460		40.92				C
	ATOM	12564	CB	VAL	С	31			47.300	23.638	57.892	1.00	37.95				С
	ATOM	12566		VAL		31			46.317	24.595	58.524	1.00	41.29				С
	ATOM	12570		VAL		31			48.718		58.132	1.00	41.26	•			С
	ATOM	12574	C	VAL		31			45.574	22.155	58.515	1.00	45.40				С
55		12575	ŏ	VAL		31			44.885		57.555		46.26				0
,,	:ATOM	12576	N	ASP					45.082		59.658		44.37				N
	MOTA:		CA	ASP			•		43.693				42.08				C
	MOTA	12578 12580	CB	ASP						19.799			48.54	٠			C
	ATOM		CG						42.270				55.02				С
60	MOTA								41.331				57.45				0
60	ATOM			1 ASP					42.035				54.56				0
	MOTA	12585	UD.	2 ASP	C	52			72.033					-			

_			_	7 O D C	32		42.996	22.030	60.996	1.00 42.96	•		С
5	ATOM	12586	C	ASP C	32		43.171	21.653	62.148	1.00 38.86			Ó
	ATOM	12587	0	ASP C			42.205	23.072	60.670	1.00 42.49			N
	MOTA	12588	N	THR C	33		41.382	23.757	61.655	1.00 34.59			С
	MOTA	12590	CA	THR C	33		41.102	25.275	61.297	1.00 40.43			C.
	MOTA	12592	CB	THR C	33		40.271	25.418	60.128	1.00 36.06	•		0
10	ATOM	12594		THR C	33			26.064	60.943	1.00 38.42			C
	ATOM	12596		THR C	33		42.332	23.151	61.903	1.00 37.84			С
	ATOM	12600	С	THR C	33		40.025		62.562	1.00 42.84			0
	MOTA	12601	0	THR C	33		39.181	23.773 21.985	61.347	1.00 39.71			N
	ATOM	12602	N	GLY C	34			21.204	61.713	1.00 45.14			C
15	MOTA	12604	CA	GLY C	34		38.621		62.634	1.00 44.20			С
	ATOM	12607	C	GLY C	34	•	38.955	20.018	62.710	1.00 44.56			0
	MOTA	12608	0	GLY C	34		38.190	19.062	63.318	1.00 39.94			N
	ATOM	12609	N	SER C	35 ·		40.102	20.086	64.357	1.00 36.97			C
	ATOM	12611	CA	SER C	35		40.490	19.124	63.768	1.00 41.17			C
20	MOTA	12613	CB	SER C	35		41.195	17.909	63.530	1.00 39.49			0.
	MOTA .	12616	OG	SER C	35		42.575	18.109	65.385	1.00 41.65			C
	ATOM	12618	С	SER C	35 -		41.423	19.799	65.259	1.00 38.82			o.
	MOTA	12619	0	SER C	35		41.747	20.986	66.384	1.00 30.62			N
	ATOM	12620	N	SER C	36		41.881	19.044		1.00 41.00			C
25	ATOM	12622	CA	SER C	36	•	42.683	19.621	67.476	1.00 30.37			č
	ATOM	12624	CB	SER C	36		41.755	19.879	68.673 68.393	1.00 34.74			ō
•	MOTA	12627	OG	SER C	36		40.776	20.894		1.00 34.74			Ċ
	MOTA	12629	C	SER C	36		43.908		67.975	1.00 46.46			ő
	MOTA	12630	0	SER C	36		44.478	19.169	69.000	1.00 34.55			N
30	MOTA	12631	N	ASN C	37		44.322	17.742	67.298	1.00 34.35			C
	ATOM	12633	CA	ASN C	37		45.511	17.024	67.723	1.00 38.23			Ċ
	ATOM	12635	CB	ASN C	-37		45.259	15.525	67.766	1.00 38.28			Ċ
	MOTA	12638	CG	ASN C	37		44.338	15.132	68.855	1.00 39.72			ő
	ATOM	12639		ASN C	37		43.120		68.681	1.00 38.23			N
35	MOTA	12640	ND2	ASN C			44.911		69.992	1.00 37.50			· c
	MOTA	12643	С	ASN C			46.674	17.175	66.771	1.00 37.34			ŏ
	MOTA	12644	0	ASN C			46.475	17.306	65.578	1.00 34.71			N
	ATOM	12645	N	PHE C			47.888	17.150	67.322	1.00 33.88			c
	MOTA	12647	CA	PHE C			49.090	17.051	66.525	1.00 33.22			c
40	ATOM	12649	CB	PHE C			50.203	17.902	67.126				.c
	MOTA	12652	CG	PHE C			51.541	17.943	66.303	1.00 37.60 1.00 37.64			c
	MOTA	12653		1 PHE C			52.748		66.931	1.00 37:04			Č
	MOTA	12655		1 PHE C			53.864		66.256	1.00 42.48			Ċ
	ATOM	12657	CZ	PHE C			53.869		64.938				Ċ
45	ATOM	12659		2 PHE C			52.742		64.307	1.00 43.17			č
	MOTA	. 12661		2 PHE C			51.573		64.979	1.00 38.37			Ċ
•	MOTA	12663	С	PHE C			49.361		66.531	1.00 30.08		•	ő
	ATOM	12664	0	PHE C	•	•	49.328		67.596				N
	MOTA		· N	ALA C			49.584		65.337				· C
50	ATOM	12667	CA				49.777						c
	MOTA		CB				48.450						c
•	ATOM		С	ALA (50.557						ő
	ATOM		.0.	ALA (50.252						, N
	ATOM			VAL (51.556				,		C
55	ATOM		CA	VAL (C 40		52.402						C
•	ATOM		CB	VAL	C 40		53.865						c
	ATOM			1 VAL	C 40		54.002						C
	ATOM			2 VAL	C 40		54.444		64.169				C
	ATOM			VAL	C 40		52.504	10.524					0
60	ATOM			VAL			52.333		63.627				
	ATOM			GLY	C 41		52.79	5 10.017	61.429	1.00 42.10			N
												•	

		.									1 00	36.51			С
5	MOTA	12693		GLY		41		3.024	8.600	61.217	1.00	45.89			c
-			С	GLY	С	41		4.331	8.220	61.900			•		Ö
•			0	GLY	C	41		5.312	8.941	61.803		41.98			N
	ATOM		N	ALA	С	42		4.368	7.083	62.591		49.43			C
	ATOM		CA	ALA	С	42		5.588	6,687	63.291		46.63			c
10	ATOM		CB	ALA.	С	42		5.434	6.999	64.733		44.75			c
10	ATOM	12706	С	ALA ·	С	42	5	5.868	5.196	63.096		50.91			0
	ATOM	12707	0	ALA	С	42	5	6.415	4.512	63.968		56.15			Ŋ
	ATOM	12708	N	ALA		43		5.494	4.714	61.923	1.00	51.91			C
	ATOM	12710	CA	ALA:		43	5	5.530	3.302	61.647		55.01		٠.	C
15	ATOM	12712	CB	ALA	С	43	5	54.578	2.588	62.522		56.93	, .		C.
10	ATOM	12716	С	ALA		43	5	55.118	3.057	60.232	1.00	59.43		•	
	ATOM	12717	ō	ALA		43	5	4.070	3.538	59.772	1.00	58.38			0
	ATOM .		N ·	PRO		44 .	5	55.971	2.315	59.555		59.53			N
•	ATOM	12719	·CA	PRO		44		55.738	1.800	58.207	1.00	57.91			C.
20 .	ATOM	12721	СВ	PRO		44	5	56.185	0.392	58.373		58.24			C
20	ATOM	12724	CG	PRO		44	ç	57.450	0.628	59.193		60.25			C .:
	MOTA	12727	CD	PRO		44		57.296	1.930	60.015		59.83			C
		12730	C	PRO		. 44		54.345	1.869	57.679		51.08		•	C .
	MOTA	12731	ō	PRO		44		53.427	1.440	58.331		42.11			0
25	MOTA	12732	N	HIS		45		54.228	2.439	56.483		51.18			N
25	MOTA	12734	CA	HIS		45		52.943	2.516	55.767		51.14			С
	MOTA	12736	CB	HIS		45	!	51.987	3.544	56.361		49.59			С
	ATOM	12739	CG	HIS		45		50.664	3.623	55.641		55.41			C
	ATOM	12739		HIS		45		50.552	4.007	54.318		50.15			N
20	ATOM	12740		HIS		45		49.280	3.983	53.961		48.42			·C
30	ATOM	12744				45		48.563	3.582	54.993		48.32			N
	MOTA		CD3	HIS	Č	45		49.401	3.351	56.058	1.00	50.46			С
	ATOM	12746	CDZ	HIS		45		53.171	2.803	54.287		51.98			C
	ATOM	12748	0	HIS		45		53.986	3.610	53.912		58.52			0
25	ATOM	12749	N	PRO		46		52.430	2.123	53.444		59.22			N
35	ATOM	12750	ĊA	PRO		46		52.535	2.244	51.977		58.93			С
	ATOM	12751	CB	PRO		46		51.381	1.382	51.492	1.00	60.36			С
	MOTA	12753	CG	PRC		46		51.169	0.420	52.553		62.16			С
	MOTA	12756	CD	PRC		46		51.412	1.141	53.851	1.00	58.40			С
40	MOTA	12759	CD	PRO		46		52.263		51.375	1.00	60.75			С
40	MOTA		0	PRO				52.429	3.742	50.152		66.57			0
-	ATOM	12763	N	PHE		47		51.820	4.582	52.146		53.51		•	\mathbf{N}_{\cdot}
	ATOM		CA	PHE		47		51.687	5.885	51.534		54.37			С
	ATOM	12766	CB	PHE				50.227	6.362			55.83			С
45	ATOM		CG	PHI				49.248	5.477		1.0	0 56.85			С
43	ATOM		CO	1 PHI				47.889	5.498		1.0	0 53.21			С
•	ATOM		CD.	1 PHI		47		47.022	. 4.712	50.358	1.0	0 58.68			C
	ATOM							47.494	3.872			0 53.11			С
	ATOM			2 PH				48.802	3.834		1.0	0 53.10			C ·
50	ATOM			2 PH				49.693	4.630		1.0	0 59.43			C
50	ATOM				EC			52.728	6.896			0 53.35			С
	ATOM				EC			52.739	8.075			0 47.38			0
	ATOM				UC			53.602				0 47.46			N
	ATOM				υς			54.627	7.217			0 48.00			С
ے ہے	ATOM							54.585	6.868			0 44.63			. C
55	ATOM				บ C			53.203	7.093			0 36.89			C
	ATOM				UC			53.226	7.095			0 32.35			С
	ATOM			1 LE				52.716	8.414			0 43.78			C
	.ATOM			2 LE				56.055	7.010			0 49.23			C
	ATOM				U C			56.512	5.888			0 51.31			0
60	ATOM				U			56.741	8.082			0 54.74			N
	MOTA	4 12803	3 N	HI	S	2 49		50.741	0.002		~				

5	ATOM	12805	CA	HIS	С	49		58.138	8.036	52.290	1.00 55.16		C	
5	ATOM	12807	CB	HIS		49		58.563	9.276	51.513	1.00 62.74		C	
	ATOM	12810	CG	HIS		49		57.851	9.479	50.216	1.00 80.32			:
	ATOM	12811		HIS		49		57.953	8.596	49.157	1.00 90.23		N	
	ATOM	12813		HIS		49		57.221	9.041	48.148	1.00 90.85		С	
10		12815		HIS		49		56.653	10.180	48.512			N	
10	MOTA	12817		HIS		49		57.032	10.477	49.799	1.00 85.66		С	
	MOTA		CDZ	HIS		49		58.985	8.110	53.491	1.00 52.56		C	
	MOTA	12819	Ö	HIS		49		60.083	7.550	53.529	1.00 57.27		О	
	MOTA	12820		ARG		50		58.495	8.859	54.472	1.00 46.86		N	
	ATOM	12821	N	ARG		50		59.152	8.928	55.749	1.00 44.15		C	
15	ATOM	12823	CA	ARG		50		60.123	10.094	55.776	1.00 47.15		C	
	MOTA	12825	CB	ARG		50		59.543	11.362	55.346	1.00 48.57		C	
	MOTA	12828	CG			50		60.498	12.504	55.358	1.00 47.15		(3
•,	MOTA	12831	CD	ARG				59.733	13.667	54.935	1.00 57.92		N	N
	MOTA	12834	NE	ARG		50		60.210	14.894	54.724	1.00 57.78		(3
20	MOTA	12836	CZ	ARG		50			15.192	54.882	1.00 51.00		ľ	N
	ATOM	12837		ARG		50		61.491	15.132	54.342	1.00 59.97			N
•	ATOM	12840		ARG		50		59.366	9.000	56.918	1.00 40.60			С
	MOTA	12843	С	ARG		50		58.192		56.762	1.00 38.05		. (0
	MOTA	12844	0	ARG		50		56.992	9.149		1.00 43.42			N
25	ATOM	12845	N	TYR		51	. •	58.746	8.873	58.107	1.00 46.93			C
	ATOM	12847	CA	TYR		51		57.961	8.988	59.304	1.00 48.86			C
	ATOM	12849	CB	TYR		51		57.068	7.774	59.414	1.00 57.25			Č
	ATOM	12852	CG	TYR		51		57.838	6.503	59.490	1.00 57.25			c
	ATOM	12853	CD1	TYR		51		58.167	5.944	60.706	1.00 53.32			c
30	ATOM	12855	CE1	TYR	С	51		58.876	4.753	60.768				c
	ATOM	12857	CZ	TYR	С	51		59.260	4.118	59.593	1.00 65.22			0
	ATOM	12858	OH	TYR		51		59.966	2.928	59.626	1.00 68.18	•		c
	ATOM	12860		TYR		51		58.939	4.662	58.380	1.00 61.62			c
	ATOM	12862	CD2	TYR	С	51		58.236	5.844		1.00 62.51			C
35	MOTA	12864	Ċ	TYR		51		58.822	9.143	60.563	1.00 40.91	.•		0
	ATOM	12865	0	TYR	C	51		59.999	8.948	60.522	1.00 42.94	•		
	ATOM	12866	N	TYR	· C	52		58.190	9.503	61.674	1.00 40.91			N
	MOTA	12868	CA	TÝR		52		58.832	9.726	62.976	1.00 40.27			C
	ATOM	12870	СВ	TYR		52		57.747	10.233	63.886	1.00 41.76			С
40	ATOM	12873	CG	TYR	C	52		58.122	10.764	65.232	1.00 41.11			C
	ATOM	12874		TYR		52		59.174	11.588	65.399	1.00 47.30			C
	ATOM	12876		LTYR		52		59.492	12.084	66.637	1.00 50.41			C
	ATOM	12878	CZ	TYR		52		58.750	11.768	67.719	1.00 49.29			С
	ATOM	12879	ОН	TYR		52		59.121	12.304	68.943	1.00 53.62			0
45	MOTA	12881		2 TYP		52		57.685	10.943	67.579				c
73	ATOM			2 TYP		52		57.377	10.449	66.340				C
•	ATOM	12885		TYF		52		59.394		63.684	1.00 41.56			С
	ATOM		ő					58.631		64.087	1.00 42.35			O
		12887	N	GLN		53		60.711			1.00 44.45			N
50			CA			53		61.404						С
50	MOTA		CB					62.681				•		С
	MOTA		CG					62.440				•		C
	ATOM							63.227			`			C
	ATOM		CD		1 C			63.842	_					0
	ATOM			1 GL				63.204						N
55	ATOM			2 GLi				61.698						С
	ATOM				N C					•				0
	ATOM				N C			62.595						N
	ATOM				G C			60.926						С
:.	ATOM				G C			61.004						c
60	ATOM				G C			59.828					•	č
,	MOTA	1 12911	. CG	AR	G C	54		58.57	8.077	68.924	T.00 40.01			_

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5	MOTA	12914	CD	ARG	С	54		57.389	7.431	69.538		39.95		С
	ATOM	12917	NE	ARG	С	54		57.137	6.168	68.844		40.64		N
	ATOM	12919	CZ	ARG	С	54		56.124	5.372	69.092		45.54		C
	ATOM	12920	NH1	ARG	С	54		55.230	5.686	70.027		47.14		N
	MOTA	12923	NH2	ARG	С	54		56.000	4.257	68.396		48.98		N
10	ATOM	12926	С	ARG		54		62.219	7.302	69.005		47.24		C
10	ATOM	12927	ō	ARG		54		62.621	7.870	70.013	1.00	49.66		0
	ATOM	12928	N	GLN		55		62.795	6.236	68.482	1.00	55.23		N
	ATOM	12930	CA	GLN		55		63.960	5.624	69.061	1.00	55.09		С
	ATOM	12932	CB	GLN		55		64.162	4.277	68.388	1.00	60.40		С
15	ATOM	12935	CG	GLN		55		64.836	4.423	67.025	1.00	62.46		С
13		12938	CD	GLN		55		63.988	4.048	65.850	1.00	61.26	•	С
	MOTA			GLN		55		64.541	3.682	64.814	1.00	62.44		0
	MOTA	12939				55		62.663	4.155	65.977		55.40		N
•	ATOM	12940		GLN				65.197	6.491	68.835		54.46		С
	ATOM	12943	C.	GLN		55				69.567		57.35	•	Ō
20	ATOM	12944	0	GLN		55		00.200	7.368	67.828		51.48		N
•	MOTA	12945	N	LEU		56		65.157		67.506		50.79		C
	ATOM	12947	CA	LEU		56		66.331	8.196			51.27	•	c
	ATOM	12949	CB	LEU		56		66.500	8.354	65.983		51.47		Č
	ATOM	12952		LEU		56		66.445	7.101	65.101		48.56		c
25	MOTA	12954		LEU		56		66.780	7.437	63.654				C
	MOTA	12958	CD2	LEU		56		67.364	6.071	65.629		47.53		
	MOTA	12962	С	LEU	С	56		66.333	9.594	68.071		46.70		C
	MOTA	12963	0	LEU	С	56		67.129	10.385	67.639		50.22		0
	ATOM	12964	N	SER	C	57		65.453	9.904	69.012		48.97		И
30	ATOM	12966	CA	SER	С	57		65.298	11.260	69.565		45.66		С
	ATOM	12968	CB	SER	С	57		63.841	11.680	69.338		44.35		С
	ATOM	12971	OG	SER	С	57		63.487	12.916	69.932		48.13		0
	ATOM	12973	С	SER	C	57		65.585	11.166	71.061		.45.21		С
•	ATOM	12974	0	SER		57		64.960	10.361	71.721		46.15		0
35	ATOM	12975	N	SER				66.513	11.955	71.608		45.62		N
	ATOM	12977	CA	SER		. 58	•	66.828	11.885	73.068	1.00	44.99		С
	ATOM	12979	СВ	SER		58		68.186	12.471	73.363	1.00	39.39		С
	ATOM	12982	OG	SER		58		68.146	13.786	72.887	1.00	39.14		0
	ATOM	12984	·C	SER		58		65.869	12:689	73.911	1.00	44.75		C.
40	ATOM	12985	ō	SER		58		65.676	12.433	75.101	1.00	48.81		0
70	ATOM	12986	N	THR		59		65.272	13.684	73.297	1.00	44.46		N
	ATOM	12988	CA	THR		59		64.320	14.493	73.998	1.00	44.45		С
		12990	CB	THR		59		64.257	15.835	73.328		39.83		С
	ATOM	12992		THR		59		63.953	15.610	71.960		44.67		0
45	ATOM	12994		THR		59		65.592	16.504	73.267		42.08		С
.43	ATOM			THR		59		62.910	13.889	73.942		49.34		С
	ATOM	.12998	C			59		61.953	14.574	74.329		60.35		0
	ATOM	12999	0	THR					12.652	73.481		45.28		N
	ATOM	13000	N	TYR				62.732	12.126	73.373		42.73	×	c
	ATOM	13002	CA	TYR		60		61.378				44.34		č
50	MOTA	13004	CB			60		61.255	11.078	72.235				č
	ATOM	13007	CG	TYP		60		60.194	10.045	72.509		39.04		Ċ
	MOTA	13008		LTYP		60		58.876	10.239	72.078		35.41		
*****	ATOM	13010		L TYP		60		57.873	9.308	72.344		37.20		C
	ATOM	13012	CZ	TYF		60		58.178	8.161	73.048		48.24		C
55	ATOM	13013	OH	TYP		60		57.188	7.246	73.312		56.91		0
	ATOM	13015		2 TYF		60		59.496	7.934	73.495		47.13		C
	ATOM		CD	2 TYF	Ç	60		60.496	8.895	73.223		35.96		C
	ATOM			TYF		60		61.040	11.487	74.690		0 47.68		C
	ATOM			TYF		60		61.858	10.721	75,189		0 47.26		Q
60	ATOM			ARC				59.843	11.823			0 48.05		N
	ATOM					61		59.216	11.303	76.438	1.0	0 46.98		С
						_								

_		10005	00	NDC.	_	6i	58.773	12.440	77.347	1.00 4	9.63	•	С
5	ATOM	13025	CB	ARG ARG		61	59.774	12.823	78.369	1.00 6	0.48		С
	ATOM	13028	CG	ARG		61	60.050	11.712	79.429	1.00 6	6.22		C
	ATOM	13031	CD	ARG		61	60.843	10.550	78.950	1.00 - 6			N
	ATOM	13034	NE	ARG		61	62.129	10.585	78.575	1.00 7			C
	MOTA	13036	CZ				62.838	11.717	78.591	1.00 7			N
10	MOTA	13037		ARG		61	62.719	9.472	78.174	1.00 7			N
	ATOM	13040		ARG		61	57.932	10.601	76.126	1.00 4			С
	MOTA	13043	С	ARG		61	57.148		75.381	1.00 4		·	0
•	MOTA			ARG		61	57.694	9.431	76.724	1.00 5			N
	MOTA	13045	N	ASP		62	56.483	8.630	76.471	1.00 5			С
15	MOTA	13047	CA	ASP		62	56.850	7.160	76.486	1.00			С
		13049	CB	ASP		62	55.795	6.279	75.881	1.00			С
	MOTA	13052	CG	ASP		62	54.599		75.822	1.00			0
	MOTA	13053		ASP		62	56.086	5.151	75.442	1.00			0
	MOTA	13054		ASP		62	55.442	8.874	77.549	1.00			C
20	ATOM	13055	С	ASP		62 62	55.779	8.845	78.699	1.00			0
	ATOM	13056	0	ASP			54.192	9.116	77.150	1.00			N
	MOTA	13057	N	LEU		63	53.075	9.402	78.057	1.00			С
	MOTA	13059	CA	LEU		63	52.160	10.437	77.404	1.00			С
	MOTA	13061	CB	LEU		63	52.776	11.820	77.240	1.00			С
25	MOTA	13064	CG	LEU		63	51.756	12.771	76.610	1.00			С
·	ATOM	13066		LEU		63	53.270	12.356	78.568	1.00			С
	ATOM	13070	•	LEU		63	52.234	8.183	78.511	1.00			С
	ATOM	13074	C	LEU		63 63	51.489	8.276	79.475		56.10		0
•	MOTA	13075	0	LEU		64	52.323	7.053	77.828		60.31		N
30	ATOM	13076	N	ARG		64	51.702	5.821	78.337		63.72		С
	MOTA	13078	CA	ARG		64	52.093	5.634	79.801		66.02		Ċ
	MOTA	13080	CB	ARC		64	53.077	4.540	80.025		71.85		С
		13083	CG	ARG		64	54.241	4.949	80.865		76.21		С
0.5	ATOM	13086	CD	ARG		64	55.478	4.473	80.255		83.39		N
·35	MOTA	13089	NE	ARG		64	55.840	4.763	79.018		86.32		С
	ATOM	13091	CZ	L ARC		64	55.045	•	78.271		87.82		N
	MOTA	13092		2 ARC		64	56.989	4.300	78.528	1.00	87.10		N
	MOTA	13095	C	ARO		64	50.204	5.790	78.293		63.01		С
40:	ATOM	13098	0	ARG		64	49.556				67.08		Ó
40	MOTA	13099 13100	N		s c	65	49.639				62.20		N
	ATOM	13100	CA		s c	65	48.203		77.021	1.00	56.21		С
	MOTA		CB		s c	65	47.742		77.559		53.38		С
	MOTA MOTA		ĊG		s c	65	46.223			1.00	61.59		С
45	ATOM				s c	65	45.772		78.771	1.00	65.72		C
45	ATOM				s c		46.070	10.201	78.354		68.02		Ċ
	ATOM				s ·C		45.991		79.492		69.89		N
	ATOM				s c		48.062		75.552		50.29		C
					s c		48.950	_		1.00	42.57		0
50	ATOM ATOM				ΥC		46.965				53.19		N
50	ATOM				Y, C		46.748				53.88		C
					Y C		45.712			1.00	55.77	•	C
	MOTA .				Y C		44.967		74.141	1.00	61.89		0
	ATOM				ΤC		45.654			1.00	52.57		N
55					T C		44.753			1.00	52.31		С
55	ATOM				TC		45.485		71.457	1.00	56.46		С
	ATOM	-		1 VA			46.912			1.00	61.44		С
	ATOM			2 VA	LC		44.798			1.00	59.86		C
	MOTA				VI C		44.32			1.00	45.56		C
60	ATOM ATOM				AL C		45.00				50.56		0
60	ATOM				(R C		43.16			3 1.00	46.81		N
	ATOR	. 1314.	,					•			•		

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5	ATOM	13147	CA	TYR C	68		42.612	7.210	68.435	1.00 49.00			С
_	ATOM	13149	CB	TYR C	68		41.772	5.909	68.608	1.00 53.23			С
	ATOM	13152	CG	TYR C	68		40.433	6.120	69.280	1.00 57.32			С
	ATOM	13153		TYR C	68		39.298	6.444	68.537	1.00 61.05			С
	ATOM	13155	CE1	TYR C	68		38.076	6.653	69.151	1.00 62.40			С
10	ATOM	13157	CZ	TYR C	68		37.980	6.524	70.533	1.00 65.60			С
10	ATOM	13158	OH	TYR C	68		36.814	6.708	71.234	1.00 73.33			Ο.
	ATOM	13160		TYR C	68		39.076	6.200	71.277	1.00 68.48	3		С
	ATOM	13162	CD2	TYR C	68		40.302	6.000	70.658	1.00 61.58	3		С
	ATOM	13164	C	TYR C	68		41.731	8.358	68.011	1.00 45.30) .		С
15	ATOM	13165		TYR C	68		41.033	8.953	68.837	1.00 41.6	5		0
15		13166	N	VAL C	69		41.749	8.698	66.735	1.00 45.33	L.		N.
	MOTA	13168	CA	VAL C	69		40.903	9.802	66.283	1.00 40.69	· ·		C
	ATOM		CB	VAL C			41.736	11.055	66.122	1.00 38.5			C
٠.	ATOM			VAL C	69		40.861	12.229	65.749	1.00 42.8			С
20.	ATOM	13172		VAL C			42.426	11.348	67.410	1.00 38.40			С
20	ATOM	13176		VAL C			40.159	9.561	64.990	1.00 38.4		•	. C
	MOTA	13180	C				40.759	9.309	63.978	1.00 36.0			0
	MOTA	13181	0	VAL C			38.837	9.625	65.047	1.00 41.0			·N
	ATOM	13182	N	PRO C			37.978	9.597	63.862	1.00 41.0			С
0.5	MOTA	13183	CA	PRO C			36.731	8.856	64.378	1.00 39.3			С
25	MOTA	13185	CB	PRO C			36.868	8.792	65.844	1.00 34.8			Ċ
	MOTA	13188	CG	PRO C				9.668	66.268	1.00 41.3			Ċ
	MOTA	13191	CD	PRO C			38.030	11.001	63.320	1.00 43.2			Ċ
	MOTA	13194	С	PRO C			37.582		64.102	1.00 41.5			ō
	MOTA	13195	0	PRO C			37.305	11.927	61.985	1:00 48.4			Ŋ
.30	ATOM	13196	N	TYR C	-		37.561	11.119		1.00 45.4			C
٠.	ATOM	13198	CA	TYR C			37.249	12.328	61.206 60.317	1.00 47.5			Č
	ATOM	13200	CB	TYR C			38.446	12.615	61.024	1.00 47.3			č
	ATOM	13203	CG	TYR C			39.761	12.912	61.636	1.00 45.0			č
	ATOM	13204		TYR C			39.997	14.125	62.268	1.00 46.1			Č
35	ATOM	13206		TYR C			41.203	14.358	62.281	1.00 42.6			č
	MOTA	13208	CZ	TYR C			42.180	13.407	62.893	1.00 42.5			. 0
	MOTA	13209	OH	TYR C			43.393	13.608	61.683	1.00 42.3			Č.
	ATOM	13211		TYR C			41.963	12.246		1.00 47.1			c
	MOTA	13213		TYR			40.770	11.993	61.062 60.270	1.00 47.1			Č
40	ATOM	13215	С	TYR C			36.034			1.00 45.8			ő
	MOTA	13216	0	TYR C			35.606	10.915	60.053	1.00 47.9			N
•	ATOM	13217	N	THR C			35.456	13.081	59.683	1.00 47.3			C.
	ATOM	13219	CA	THR C			34.356	12.805	58.760	1.00 45.1			Č
	MOTA	13221	CB	THR C			34.027	14.021	57.966	1.00 40.3			. 0
45	MOTA	13223		L THR C			33.809	15.111	58.867	1.00 39.1			Ċ
	MOTA	13225		2 THR C			32.706	13.846	57.309	1.00 46.1			c
	MOTA	13229	С	THR (34.709	11.612	57.857				Ö
	MOTA	13230	0	THR C			33.884	10.719	57.657				N
	ATOM	13231	N	GLN (35.919	11.612	57.302	1.00 47.7			
50	ATOM	13233	CA	GLN (36.473	10.435	56.643				Ċ
	MOTA	13235	CB	GLN (36.522	10.536	55.123				
	ATOM	13238	CG	GLN (C 73		35.190	10.873	54.510				C
	MOTA	13241	CD	GLN (C 73			9.825					C
	MOTA	13242	OE:	1 GLN	c 73		34.197	10.163	52.435				0
55	ATOM	13243	NE:	2 GLN (C 73		34.701	8.555	53.939				N
	ATOM		С	GLN (37.866	10.291	57.206				C
	ATOM	_	0	GLN (38.559	11.293	57.431				0
	MOTA		N	GLY (38.274	9.049					N
	ATOM		CA				39 .6 16	8.758					C
60	ATOM		С	GLY,		,	39.679	8.620					C
	ATOM		0	GLY			38.937	9.283	60.166	1.00 46.	21		0
			_		•								

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5	ATOM	13255	N	LYS C	75		0.548	7.729	59.907	1.00 42				N
	ATOM	13257	CA	LYS C	75	•	0.894	7.639	61.306	1.00 40				С
	MOTA	13259	CB	LYS C	75	3	9.809	6.919	62.124	1.00 48				С
	ATOM	13262	CG	LYS C	75	3	39.614	5.420	61.883	1.00 48				С
	ATOM	13265	CD	LYS C	75	. 3	88.232	4.997	62.417	1.00 56				C
10	ATOM	13268	CE	LYS C	7 5	3	37.077	5.271	61.414	1.00 56				С
	ATOM	13271	NZ	LYS C	75	3	36.653	4.074	60.594	1.00 52				N
	ATOM	13275	С	LYS C	75	4	12.270	6.970	61.410	1.00 41				C
	ATOM	13276	0	LYS C	75	4	12.739	6.338	60.471	1.00 36				0
	ATOM'	13277	N	TRP C	76	4	12.928	.7.114	62.547	1.00 40				Ŋ
15	MOTA	13279	CA	TRP C	76		14.226	6.491	62.759	1.00 41				С
•	ATOM	13281	CB	TRP C	76	4	15.383	7.434	62.347	1.00 46				C
	ATOM	13284	CG	TRP C	.76	4	15.243	8.876	62.701	1.00 48				C
	ATOM	13285	CD1	TRP C	76		44.953	9.877	61.845	1.00 52				C
	MOTA	13287	NE1	TRP C	76	4	14.909	11.087	62.505	1.00 48				N
20	ATOM	13289	CÉ2	TRP C	76		45.183	10.869	63.828	1.00 35				C
	ATOM	13290		TRP C	76		45.401	9.492	63.992	1.00 46				С
	ATOM	13291	CE3	TRP C	76		45.705	9.007	65.273	1.00 46				С
<i>:</i> ·	ATOM	13293		TRP C	76		45.773	9.884	66.311	1.00 41				С
	ATOM	13295		TRP C	76		45.548	11.258	66.099	1.00 43				С
25	ATOM	13297		TRP C	76		45.254	11.751	64.859	1.00 38	.46			C.
20	MOTA	13299	С	TRP C	76		44.298	6.196	64.227	1.00 41				C.
	ATOM	13300	0.	TRP C	76		43.547	6.756	65.015	1.00 44				0
•	ATOM	13301	N	GLU. C	77		45.182	5.313	64.634	1.00 45	.94			N
	ATOM	13303	CA	GLU C	77		45.296	5.053	66.052	1.00 48	3.17			C
30	ATOM	13305	CB	GLU C	7.7	-	44.775	3.663	66.408			•		С
50	ATOM	13308	CG	GLU C	77		44.214	3.526	67.827	1.00 59				C,
	ATOM	13311	CD	GLU C	77		43.153	2.429	67.948	1.00 63	3.65			С
	ATOM	13312		GLU C	77		42.966	1.729	66.889	1.00 61	.90			. 0 ·
	ATOM	13313		GLU C	77		42.540	2.277	69.099	1.00 6	L.88			0
35	ATOM	13314	С	GLU C	77		46.744	5.240	66.353	1.00 44	1.15			Ċ
	ATOM	13315	0	GLU C	77		47.580	5.038	65.481	1.00 50	71			0
	MOTA	13316	N	GLY C	78		47.044	5.661	67.572	1.00 4				N
	ATOM	13318	CA	GLY C	78		48.423	5.866	67.994	1.00 4				С
	ATOM	13321	С	GLY C	78		48.639	5.842	69.506	1.00 4			-	C
40	ATOM	13322	0	GLY C	78		47.757	5.539	70.298	1.00 5		•		0
	ATOM	13323	.N	GLU C	79		49.850	6.195	69.897	1.00 4				N
•	ATOM	13325	CA	GLU C	79		50.272	6.234		1.00 4				С
	MOTA	13327	CB	GLU C	79		51.404	5.178	71.418	1.00 5				С
	MOTA	13330	CG	GLU C	79		51.511	4.299	70.145	1.00 5				C
45	ATOM	13333	CD	GLU C	79		52.118	2.920	70.337	1.00 6				С
	ATOM	13334	OE1	GLU C	79		51.371	1.881	70.186	1.00 6				0
	MOTA	13335	OE2	GLU C	79		53.349	2.881	70.607	1.,00 6				0
	ATOM	13336	C.	GLU C	79		50.759	7.688	71.503					C
	ATOM		0	GLU C			51.353	8.279	70.596	1.00,4				Ó.
50	ATOM	13338	N.	LEU C			50.507	8.280	72.669					N.
	ATOM	13340	CA	LEU C	.80		50.942	9.647	72.904	1.00 3				С
	ATOM	13342	CB	LEU C			50.042	10.306	73.887	1.00 4			٠.	Ç
	ATOM	13345	CG	LEU C	80		48.580	10.390	73.740					· C
	ATOM	13347	CD1	LEU C	80		48.100	10.134	75.134					С
55	MOTA	13351	CD2	LEU C	80		48.212	11.816	73.219					С
	ATOM	13355	C	LEU C			52.283	9.789					,	C
	ATOM	13356	0	LEU C			52.812	8.841						0
	ATOM	13357	N	GLY C			52.791		73.540					N
	ATOM	13359		GLY C		•	54.096							С
60	ATOM			GLY C			54.408		73.856					С
	ATOM	13363		GLY C			53.588			1.00 4	1.07			. 0
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5	MOTA	13481	NE2	HIS	C	89		61.528	26.610	54.196	1.00 56.97			N
	MOTA	13483	CD2	HIS	С	89		60.368	26.521	54.928	1.00 59.06			C
	MOTA	13485	С	HIS	С	89		58.422	29.176	58.631	1.00 50.27			C
	MOTA	13486	0	HIS	С	89		57.299	29.343	58.186	1.00 51.95			0
	MOTA	13487	N	GLY	С	90		58.780	29.525	59.865	1.00 51.98			N .
10	MOTA	13489	CA .	GLY	С	90		57.866	30.031	60.882	1.00 49.95			C
	MOTA	13492	С	GLY		90		58.685	30.687	61.980	1.00 47.79			C
	MOTA	13493	Ο.	GLY	С	90		59.913	30.701	61.889	1.00 57.85			0
	ATOM	13494	N	PRO		91	,	58.029	31.167	63.034	1.00 42.33		•	N
	MOTA	13495	CA	PRO		91		58.688	32.056	63.990	1.00 45.30			C.
15	MOTA	13497	CB	PRO	С	91		57.586	32.447	64.952	1.00 43.17			C
	MOTA	13500	CG	PRO	С	91		56.415	31.674	64.623	1.00 41.44			C
	ATOM	13503	CD	PRO	С	91		56.658	30.820	63.433	1.00 45.00			C
	ATOM	13506	С	PRO	С	91		59.751	31.213	64.620	1.00 48.09			C
	ATOM	13507	0	PRO	С	91		59.535	30.024	64.624	1.00 54.44			0
20	MOTA	13508	N	GLN	С	92		60.843	31.737	65.131	1.00 53.59			N
	MOTA	13510	CA -	GLN	С	92		61.921	30.814	65.443	1.00 59.67			C
	MOTA	13512	CB	GLN	С	92		63.309	31.354	65.139	1.00 62.99			C
	ATOM	13515	. CG	GLN	С	92		63.355	32.565	64.259	1.00 69.98			C
	MOTA	13518	CD	GLN	·C	92		64.686	32.618	63.546	1.00 76.93			C
25	ATOM	13519	OE1	GLN	C	92		65.246	31.554	63.191	1.00 79.49			0
	ATOM	13520	NE2	GLN	С	92		65.210	33.837	63.335	1.00 74.23			N.
	ATOM	13523	С	GLN	С	92		61.893	.30.449	66.851	1.00 59.04			С
	ATOM	13524	0	GLN	C	92		62.643	30.978	67.638	1.00 67.08			0
	ATOM	13525	N	VAL	С	93		61.035	29.507	67.152	1.00 57.44			N
30	ATOM	13527	CA	VAL	С	93		60.894	29.057	68.483	1.00 58.21			C
	ATOM	13529	CB	VAL	С	93		59.535	29.387	68.986	1.00 60.39			C
	ATOM	13531	CG1	VAL	C	93		59.427	30.878	69.168	1.00 64.36			C.
	MOTA	13535	CG2	VAL	С	93		58.494	28.878	68.008	1.00 60.84			C.
	ATOM	13539	С	VAL	·C	93		61.032		68.473	1.00 59.93			C
35	ATOM	13540	0	. VAT	С	93		61.183	26.945	67.436	1.00 63.78			0
-	ATOM	13541	N	THR	·C	94		60.970	27.039	69.664	1.00 60.01			N
	MOTA	13543	CA	THR		94		61.045	25.637	69.862	1.00 58.54			C.
	· ATOM	13545	CB	THR		94		62.448	25.299	70.252	1.00 59.14			C
	ATOM	13547		THR		94		63.337	26.190	69.577	1.00 65.27			C
40	ATOM	13549		THR		94		62.847	23.941	69.736	1.00 60.54			C.
	MOTA	13553	С	THR		94		60.123	25.447	71.023	1.00 59.67			o
	MOTA	13554	. 0	THR		94		60.260	26.139	72.029	1.00 64.36			N
	MOTA	13555	N	VAL		95		59.170	24.539	70.905	1.00 55.96			C
	MOTA	13557	CA	VAL		95		58.299	24.281	72.036	1.00 52.71			C
45	MOTA	13559	CB	VAL		95		56.881		71.815	1.00 49.07 1.00 53.95			c
	ATOM '			VAL		95		56.947	26.091	71.056	-			c
	ATOM	13565		VAL		95		56.065	23.897	71.054	•			C
	MOTA	13569	C			.95		58.193		72.218	1.00 48.65 1.00 52.66			ŏ
	MOTA	13570		VAL		.95		58.321	22.079	71.264	1.00 48.25			N
50	MOTA	13571	N	ARG		96		57.955	22.378	73.446				C
	MOTA	13573		ARG		96		57.728	20.980	73.704	1.00 44.23			Ċ
	MOTA	13575		ARG		.96		58.145	20.582	75.105	1.00 43.93			c
	MOTA	13578	CG	ARG		96		57.739	19.139	75.427	1.00 45.83			c
	MOTA	13581	CD	ARG		96		58.485	18.481	76.591	1.00 44.68			N
55	MÒTA	13584	NE	ARG		96		59.906	18.368	76.346				C
	ATOM	13586	CZ	ARG		96		60.516	17.279	75.875	•			N
	ATOM			ARG				59.848	16.181	75.591				N
	MOTA	13590		2 ARG				61.827	17.292	75.698				C
	MOTA		C	ARG				56.242	20.824	73.546				Ö
60		13594	0	ARG				55.491	21.695	74.008				N
	ATOM	13595	N	ALA	J C	97		55.813	19.729	72.908	1.00 43.97	1		14

	•				•						•			
5	ATOM	13597	CA	ALA C	97		54.388	19.518	72.622	42.35				С
•	ATOM	13599	CB	ALA C	97		54.060	20.108	71.278	42.11				С
	ATOM	13603	С	ALA C	97		53.894	18.105	72.636	 40.41				С
	MOTA	13604	0	ALA C	97		54.575	17.166	72.319	51.69				0
	ATOM	13605	N	ASN C	98		52.651	17.957	72.994	46.04				N
10	ATOM	13607	CA	ASN C	98		52.017	16.668	72.887	 44.67				С
	ATOM	13609	CB	ASN C	98		50.544	16.823	73.230	44.47				С
	ATOM	13612	CG	ASN C	98		50.342	17.320	74.619	44.86				C
	ATOM	13613	OD1	ASN C	98		50.884	16.760	75.563	46.18				Ο.
	MOTA	13614	ND2	ASN C	98		49.564	18.378	74.762	48.48				Ņ
15	ATOM	13617	С	ASN C	98		52.175	16.171	71.463	 41.60				C
	MOTA	13618	0	ASN C	98		52.201	16.957	70.538	39.27				O
	MOTA	13619	N	ILE C	99		52.269	14.866	71.286	41.90				N
	ATOM	13621	CA	ILE C	99		52.403	14.307	69.954	46.94				С
•	ATOM	13623	CB	ILE . C	99	•	53.861	14.330	69.470	41.20				С
20	ATOM	13625	CG1	ILE C	99		54.362	15.744	69.192	46.97				С
-	ATOM	13628	CD1	ILE C	99		55.885	15.841	68.773	44.25				C
•	MOTA	13632	CG2	ILE C	99		53.939	13.652	68.168	45.91				C
	ATOM	13636	C	ILE C	99		51.914	12.870	69.953	47.27				Ç
	MOTA	13637	0	ILE C	99		52.407	12.081	70.711	58.57				0
25	ATOM	13638	N	ALA C	100		50.944	12.554	69.116	46.89				N
	ATOM	13640	CA	ALA C	100		50.418	11.219	68.962	46.93				С
	ATOM	13642	CB	ALA C	100		48.949	11.274	68.540	45.92				С
	ATOM	13646	С	ALA C	100		51.197	10.514	67.884	48.45				С
	ATOM	13647	0	ALA C	100		51.172	10.906	66.711	45.06				0
30	ATOM	13648	N	ALA (101		51.872	9.436	68.250	47.39				N
	ATOM	13650	CA	ALA (101		52.639	8.732	67.260	46.43				C
	ATOM	13652	CB	ALA (101		53.820	8.041	67.940	47.14				C
	MOTA	13656	C.	ALA (101		51.690	7.749	66.604	41.79				С
	ATOM	13657	0	ALA (2 101		51:118	6.968	67.307	48.05	• •			0
35	MOTA	13658	N		102	-	51.500	7.781	65.285	42.66				N
	ATOM	13660	CA		102		50.507	6.878	64.635	42.52				Ç
•	MOTA	13662	CB		102		49.916	7.478	63.366	37.68				Ċ
	ATOM	13664		ILE (49.273	8.809	63.646	42.95				. C
	ATOM	13667		ILE (49.029	9.597	62.382	48.42		,		, C C
40 · .	MOTA	13671		ILE (48.845	6.590	62.789	42.11				c
	MOTA	13675	С		C 102		51.141	5.609	64.183	42.17				0
	MOTA	13676	0		C 102		52.146	5.671	63.469 64.581	50.97				N
•	MOTA	13677	N		C 103		50.529	4.493		 38.74				C
4.5	MOTA	13679	CA		C 103		50.950	3,.130	64.257 65.542	31.31				č
45	ATOM	13681	CB		C 103		51.024	2.324	66.252	37.91				Ö.
	MOTA	13683			C 103		49.802	2.511	66.443	25.93				Ċ
	ATOM	13685			C 103		51.988	2.821 2.306	63.434	44.91				Ċ.
	MOTA	13689	C		C 103		49.936		63.067	49.83				0.
50	ATOM	13690	0		C 103		50.222	1.153	63.161	50.27			1	N
50	MOTA	13691	N		C 104		48.764	2.866	62.535	52.57				c
	MOTA	13693	CA		C 104		47.674	2.128	63.591	58.34				c
	ATOM	13695	CB		C 104		46.967		63.935	69.41				c
	ATOM	13698	CG		C 104		47.546	-0.048	64.324	78.52				C
EF	ATOM	13701	CD		C 104		46.428	-0.983	64.642	80.85				ŏ
55	ATOM	137.02			C 104		45.341	-0.435	64.313	82.93				ŏ
	ATOM	13703			C 104 C 104		46.629	-2.229 3.068	62.052	48.07				-C
	ATOM	13704	C		C 104		46.607 46.134	3.888	62.835	35.83				ő
	ATOM	13705	0		C 104		46.134	2.970		49.78				N
60	ATOM	. 13706	N.		C 105		45.155	3.896		51.92				c
60	ATOM	13708	CA	-				5.173	59.821	48.19				Č
	ATOM	13710	CB	, SER	C 105		45.802	J.113	JJ . U . L	 	•			_

5	ATOM	13713	OG	SER C	: 105	46.446	4.896	58.587	1.00 50.41			0
	ATOM	13715	С	SER C	105	44.336	3.307	59.195	1.00 53.97			С
	MOTA	13716	0	SER C		44.748	2.324	58.583	1.00 54.52			0
	MOTA	13717	N	ASP C		43.190	3.933	58.931	1.00 48.85			N
	MOTA	13719		ASP C		42.327	3.568	57.825	1.00 54.43			С
10	MOTA	13721	CB	ASP C		41.117	2.695	58.274	1.00 53.40			C
	MOTA	13724	CG	ASP C		40.419	1.971	57.076	1.00 59.23			С
	MOTA	13725	OD1	ASP (106	41.164	1.374	56.243	1.00 60.96			0
	MOTA	13726	OD2	ASP C	106	39.146	1.940	56.861	1.00 64.74			0
	ATOM	13727	С	ASP C	106	41.882	4.891	57.127	1.00 53.64			С
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00	ATOM	13822			C 111		5.837	45.099	1.00 65.39			N
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	MOTA	14052	С	ALA C 127		40.708	15.676	71.871	1.00 53.51			C	
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10	ATOM	14054	N	ARG C 128		41.570	14.700	71.591	1.00 53.29			-N	
•	MOTA	14056	CA.	ARG C 128		41.396	13.345	72.102	1.00 50.59			C	
	MOTA	14058	CB	ARG C 128		41.159		70.949	1.00 57.97		•	C	
	MOTA	14061	CG	ARG. C 128		39.759	12.300	70.183	1.00 59.94			C	
	ATOM	14064	CD	ARG C 128		38.475	12.155	71.017	1.00 69.66			C	
15	MOTA	14067	NE	ARG C 128		37.271	12.355	70.198	1.00 76.55			. И	
	MOTA	14069	CZ	ARG C 128		36.442	11.399	69.770	1.00 84.49			C	
	MOTA	14070		ARG C 128		36.641	10.106	70.062	1.00 85.61			N	
_	MOTA	14073		ARG C 128		35.389	11.753	69.034	1.00 86.88			N C	
	ATOM-	14076	С	ARG C 128		42.707	13.008	72.850	1.00 50.92			0	
20	ATOM .	14077	0	ARG C 128		43.799		72.544	1.00 47.14	•		· N	
	MOTA	14078	N	PRO C 129		42.662		73.847	1.00 45.26 1.00 42.08			C	
	ATOM	14079	CA	PRO C 129		41.469	11.450	74.333				Ċ	
•	ATOM		. CB	PRO C 129		42.028	10.478	75.365	1.00 43.25 1.00 38.09			Ċ	
	ATOM	14084		PRO C 129		43.561	10.579	75.290	1.00 35.38			C	
25	MOTA	14087	CD	PRO C 129		43.892	11.844	74.590	1.00 33.38	·			
	MOTA	14090	С	PRO C 129		40.487	12.337	75.054 75.129	1.00 49.13			Ċ	
	ATOM	14091	0	PRO C 129		39.322	11.949	75.578	1.00 52.35			N	
	ATOM	14092	N	ASP C 130		40.919	13.483 14.394	76.283	1.00 55.40			Ċ	
	MOTA	14094		ASP C 130		40.023 39.774	13.858	77.664	1.00 61.87			Č	
30	MOTA	14096	CB	ASP C 130 ASP C 130		41.048	13.867	78.498	1.00 70.21			Ò	
	MOTA	14099	CG	ASP C 130		41.533	12.794	78.934	1.00 73.11		. •	Ċ	
	ATOM	14100 14101		ASP C 130		41.650	14.930	78.752	1.00 74.28			C)
	MOTA MOTA	14101	C	ASP C 130		40.659	15.766	76.453	1.00.55.47			(3
35	ATOM	14102	ō	ASP C 130		41.857	15.911	76.312	1.00 47.00			()
33	ATOM	14103	N	ASP C 131		39.835	16.755	76.804	1.00 60.76			ł	1
	ATOM	14106	CA	ASP C 131		40.235	18.173	76.853	1.00 58.88			(
	ATOM	14108	CB	ASP C 131		39.051	19.107	77.223	1.00 63.07				C
	ATOM	14111	CG	ASP C 131		38.290	18.660	78.474	1.00 72.14			(
40	ATOM	14112		ASP C 131		38.685	17.632	79.058	1.00 82.97	. · · ·			0
	ATOM	14113	OD2	ASP C 131		37.281	19.261	78.948	1.00 76.88				0
	ATOM	14114	C	ASP C 131		41.415	18.554	77.696	1.00 52.31				С
	ATOM	14115	Ο.	ASP C 131	• '	41.698	19.728	77.795	1.00 60.98	•			0
-	ATOM	14116	N	SER C 132		42.116	17.620	78.304	1.00 47.46				N
45	ATOM	14118	CA	SER C 132		43.311	17.999	79.054	1.00 45.98				C.
•	ATOM	14120	CB	SER C 132		43.450	17.206	80.331	1.00 46.66				С
	MOTA	14123	OG	SER C 132		42.859	15.924	80.195	1.00 49.20				0
	ATOM	14125	С	SER C 132		44.574	17.843		1.00 47.95				С
	MOTA	14126	0	SER C 132		45.649	18.235	78.650	1.00 52.86				0
50	ATOM	14127	N	LEU C 133		44.449	17.292						N
	ATOM	14129	CA	LEU. C 133		45.591	17.140	76.156	1.00 47.27				C
	ATOM	14131	CB	LEU C 133		45.366			1.00 46.70		•		C
	MOTA	14134	CG	LEU C 133		46.663			1.00 48.65	• •			C
	ATOM	14136		LEU C 133		47.713							C
55	MOTA	14140		LEU C 133		46.539			1.00 50.53				C
•	MOTA	14144	С	LEU C 133		45.821	18.432		1.00 50.94				C O
	ATOM	14145	0	LEU C 133		45.405			1.00 58.31 1.00 51.70				N.
	ATOM	14146	N	GLU C 134		46.478							C
	MOTA	14148	CA	GLU C 134		46.764							C
60	ATOM	14150	CB	GLU C 134		47.967 48.225							C
	MOTA	14153	CG	GLU C 134		40.223	22.140	10.500	1.00 33.32				•

		•					٠ .	•					
5	ATOM	14156	CD (GLU C 134		49.438	23.242	76.750		65.65			C
3	ATOM	14157		GLU C 134		49.225	23.685	77.918		66.55			0
	ATOM	14158		GLU C 134		50.605	23.183	76.240		53.92			0
	MOTA	14159		GLU C 134		47.099	20.439	73.944		55.09			C
	MOTA	14160		GLU C 134		47.972	19.634	73.636	1.00	51.08			0
10	MOTA	14161	-	PRO C 135		46.399	21.161	73.042		52.45			N
10.	ATOM	14162		PRO C 135		46.789	21.308	71.624		47.35			С
	ATOM			PRO C 135		45.590	22.018	71.001	1.00	44.20			C
	ATOM	14167		PRO C 135		44.524	21.918	71.952		43.96			C .
	ATOM	14170		PRO C 135		45.135	21.861	73.310		48.87			С
15	ATOM	14173		PRO C 135		48.011	22.197	71.412		45.97		٠	С
13	ATOM	14174		PRO C 135		48.341	23.014.	72.238		57.63			0
	ATOM	14175		PHE C 136 .		48.665	22.030	70.271		49.91			N
	ATOM	14177		PHE C 136		49.918	22.693	69.912		41.68			C
•	ATOM	14179		PHE C 136		50.230	22.292	68.497		41.45			С
20 .	ATOM	14182		PHE C 136		51.358	23.034	67.882		41.29			C
.20	ATOM	14183		PHE C 136		52.621	22.527	67.912	1.00	37.45			С
	ATOM	14185		PHE C 136		53.646	23:172	67.368		39.54			C
	MOTA	14187		PHE C 136.		53.450	24.324	66.769		46.69			· C
	ATOM	14189	CE2	PHE C 136		52.202	24.861	66.706		47.06			C
25	ATOM	14191		PHE C 136		51,152	24.216	67.266	1.00	44.15			C
23	MOTA	14193	c	PHE C 136		49.917	24.200	69.976		48.49			C.
<i>:</i> .	ATOM	14194		PHE C 136		50.837	24.807	70.537		57.13			0
	MOTA	14195	N	PHE C 137		48.902	24.838	69.403		50.04		٠	N
	ATOM	14197		PHE C 137		48.879	26.300	69.407		42.38			C
30	ATOM	14199	СВ	PHE C 137		47.751	26.868	68.559		43.63			C
50	ATOM	14202	CG	PHE C 137		48.105	28.174	67.943		44.76			С
	ATOM	14203		PHE C 137		48.912	28.224	66.849°		48.03			C
	ATOM	14205		PHE C 137		49.260	29.420	66.290		46.54			C
	ATOM	14207	CZ	PHE C 137		48.814	30.560	66.820		44.20			C
35	ATOM	14209		PHE C 137		48.001	30.536	67.920		43.29			С
33	ATOM	14211		PHE C 137		47.648	29.358	68.474		48.04			C
	ATOM	14213	С	PHE C 137		48.782	26.775	70.830		45.85			C
	ATOM	14214	0	PHE C 137		49.389	27.784	71.210		43.40			. 0
	ATOM	14215	N	ASP C 138		48.034	26.044	71.651		46.65			N
40	ATOM	14217	CA	ASP C 138		47.918	26.481	73.024		48.49			C
	MOTA	14219	CB	ASP C 138		47.010		73.849		50.42			c
	ATOM	14222	CG	ASP C 138		45.550	25.771	73.523		56.72			o
	MOTA	14223		ASP C 138		44.771	26.066			57.59			Ö
	ATOM	14224	OD2	ASP C 138		45.080	25.619			63.56			c
45	ATOM	. 14225	С	ASP C 138		49.321	26.472			49.79		•	ő
	ATOM	14226	0	ASP C 138		49.664	27.377			50.18			N
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	· ATOM	14231	CB	SER C 139		52.080	23.926			0 42.34			.0
50	ATOM	14234	OG	SER C 139		51.244				0 38.35			č
:	ATOM	14236	С	SER C 139		52.359				0 45.80			o.
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	ATOM	14245		LEU C 140		53.654				0 46.32			c
	ATOM	14247		L LEU C 140		55.129				0 49.60		٠	c
	.ATOM		CD2	2 LEU C 140		53.172				0 46.89			Ċ
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60	MOTA	14256		LEU C 140		53.989				0 55.86			N
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	ATOM	14501	С	CYS C 155	45.685	28.565	45.895	1.00 59.52		C
	ATOM	14502	0	CYS C 155	46.576	27.824	45.515	1.00 59.33		0
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	ATOM	14508	С	GLY C 156	44.971	27.693	43.359	1.00 71.96		C
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:	ATOM	14514	СВ	ALA C 157	47.022	25.831	40.962	1.00 75.63		С
•	ATOM	14518	С	ALA C 157	45.458	27.645	40.467	1.00 79.16		C
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20.	ATOM	14525	C	GLY C 158	43.851	26.802	38.095	1.00 86.22		С
	ATOM	14526	0	GLY C 158	43.962	27.338	36.995	1.00 88.16		0
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23	ATOM	14534	CG	PHE C 159	46.710	25.287	36.552	1.00 92.61		С
	ATOM	14535		PHE C 159	46.993	26.621	36.810	1.00 92.40		. C
	MOTA	14537		PHE C 159	48.259	27.023	37.155	1.00 93.74		С
	ATOM	14539	CZ	PHE C 159	49.284	26.084	37.244	1.00 96.27		C
30	ATOM	14541		PHE C 159	49.017	24.741	36.984	1.00 95.81		С
50	ATOM	14543		PHE C 159	47.728	24.349	36.637	1.00 93.97		C .
	ATOM	14545	C	PHE C 159	45.035	23.300	38.180	1.00 94.38		С
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	ATOM	14955	С	TEO C		37.879	43.128	57.610	1.00	48.87			С
	ATOM	14956	0	LEU C	188	37.694	44.169	58.250	1.00	48.46			0
10	ATOM	14957	N ·	TRP C	189	36.971	42.152	57.523	1.00	50.27			N
•	ATOM	14959.	CA	TRP C	189	35.720	42.206	58.282	1.00	16.66			С
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	ATOM	14964	CG	TRP C	189	34.218	43.331	56.642	1.00	16.43			С
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15	ATOM	14967		TRP C		34.226	44.953	55.103	1.00 4	15.63			N
	MOTA	14969	CE2	TRP C	189	33.316	45.334	56.048	1.00 4	12.21			С
	ATOM	14970	CD2	TRP C	189	33.282	44.328	57.024	1.00 4	16.72			C
. •	MOTA	14971	CE3	TRP C	189	32.415	44.487	58.110	1.00 5	51.29			С
_	MOTA	14973		TRP:C		31.629	45.612	58.171	1.00 4	15.32			С
20	MOTA	14975	CH2	TRP C	189	31.691	46.580	57.183	1.00 4	13.31			С
	ATOM	14977	CZ2	TRP C	189	32.530	46.459	56.118	1.00 4	10.90	•		С
	ATOM	14979	С	TRP C		35.739	41.024	59.234	1.00 4	17.48			C
	ATOM	14980	0	TRP .C	189	36.164	39.955	58.850	1:00 5	52.47			0
	MOTA	14981	N	TYR C	190	35.285	41.212	60.466	1.00 4	17.80			N
25	MOTA	14983	CA	TYR C	190	35.345	40.164	61.477	1.00 4	19.62			С
	ATOM	14985	CB	TYR C	190	36.104	40.623	62.725	1.00 5	51.24			С
	ATOM	14988	CG	TYR C		37.5 69.	40.940	62.541	1.00 5	64.91			С
	ATOM	14989		TYR C		37.958	42.213	62.201	1.00 5	64.91			С
	ATOM	14991		TYR C		39.281	42.539	62.037	1.00 5	55.50			С
30	ATOM	14993	CZ	TYR C		40.257	41.593	62.212	1,00 €	50.48			С
	ATOM	14994		TYR C		41.560	42.025	62.025	1.00 €	3.65			0
	ATOM	14996		TYR C		39.909	40.309	62.557	1.00 5	4.45			С
	ATOM	14998		TYR C		38.560	39.991	62.724	1.00 5	1.81			С
	ATOM	15000	С	TYR C		33.974	39.656	61.943	1.00 5	0.65			С
35	ATOM	15001	0	TYR C		33.088	40.459	62.254	1.00 4		•		O
	ATOM	15002	N ·	THR C		33.820	38.322	61.995	1.00 4				N
•	ATOM	15004	CA	THR C		32.600	37.689	62.484	1.00 4				C
	ATOM .	15006	CB	THR C		32.090	36.647	61.492	1.00 4	13.53			С
40	ATOM	15008		THR C		30.809	36.160	61.917	1.00 4				0
40	ATOM	15010		THR C		32.973	35.419	61.505	1.00 4				С
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	MOTA	15015	0	THR C		34.143	36.540	63.858	1.00 4				0
	MOTA	15016	N	PRO C		32.125	36.948	64.774	1.00 4				N
45	ATOM ATOM	15017	CA	PRO C		32.486	36.382	66.084	1.00 4				С
43	ATOM	15019 15022	CB	PRO C		31.334	36.786	66.980	1.00 3				С
	ATOM	15025	CG CD	PRO C		30.531	37.704	66.212	1.00 3				С
	ATOM		_	PRO C		30.718	37.376	64.766	1.00 4				С
	ATOM	15028 15029	C	PRO C		32.515	34.907	66.109	1.00 4				С
50	ATOM	15029	0	PRO C		31.684	34.307	65.446	1.00 4				0
50	ATOM		N			33.444	34.335	66.868	1.00 4				N
	ATOM	15032 15034	CA CB	ILE C		33.504	32.886	67.059	1.00 4				С
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	ATOM	15036		ILE C		35.908	32.688	66.353	·1.00 4				С
55	ATOM	15043		The C		37.370	32.489	66.806	1.00 4				С
55	ATOM	15043	C	ILE C		34.900	30.990	67.792	1.00 5				С
	ATOM	15047		ILE C		32.481	32.601	68.140	1.00 4				C
	ATOM	15048	O N	ARG C		32.546	33.112	69.244	1.00 5				0
	ATOM	15051	CA	ARG C		31.515 30.380	31.789 31.515	67.788	1.00 5				N
60	ATOM	15051	CB	ARG C		29.397		68.636	1.00 5				C
	ATOM	15056	CG	ARG C		28.155	30.664 30.427	67.867	1.00 5				C
	011	10000	- G	ınıa C	#J3	~0.T))	JU.421	68.634	1.00 5	4.20		(С

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27.064
                                                      67.810 1.00 52.92
                                             29.819
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                      ARG C 194
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                                              29.795
                                                      68.558
                                    25.825
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                       TYR C 199
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                                                               1.00 44.07
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                                              27.933
                                                       63.758
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                  CB
                       TYR C 199
                                      38.494
                                              28.044
                                                       64.448 1.00 37.70
           15164
                   CG
                       TYR C 199
     MOTA
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5	ATOM	15165	CD1 5	TYR C 199		39.421	27.041	64.346	1.00 40.50		С
•	ATOM	15167		TYR C 199		40.637	27.114	65.007	1.00 42.66		С
	ATOM	15169		TYR C 199		40.932	28.211	65.793	1.00 44.12		С
	ATOM	15170		TYR C 199		42.147	28.239	66.426	1.00 35.21		0
	ATOM	15172		TYR C 199		40.008	29.247	65.931	1.00 37.43		С
10	MOTA	15174		TYR C 199		38.800	29.152	65.263	1.00 40.32		С
	ATOM	15176		TYR C 199		34.647	27.733	64.200	1.00 46.28		С
	MOTA	15177		TYR C 199		34.443	27.731	62.985	1.00 45.68		0
	ATOM	15178		GLU C 200		33.685	27.902	65.104	1.00 48.83		N
	ATOM	15180		GLU C 200		32.273	27.958	64.746	1.00 49.81	•	Ç
15	ATOM	15182		GLU C 200		31.387	27.454	65.917	1.00 51.32		С
15	ATOM	15185		GLU C 200		29.895	27.584	65.613	1.00 55.33		С
	ATOM	15188		GLU C 200		28.906	26.930	66.581	1.00 53.36		С
•	ATOM	15189		GLU C 200		29.287	26.452	67.656	1.00 54.60		0
•	ATOM	15190	OE2	GLU C 200		27.691	26.914	66.248	1.00 53.86		0
20		15191		GLU C 200		31.860	29.363	64.350	1.00 51.65		С
20	ATOM	15191	_	GLU C 200		32.292	30.315	64.973	1.00 50.64		0
	ATOM	15192		VAL C 201		31.026	29.467	63.307	1.00 51.45		N .
	ATOM	15195		VAL C 201		30.461	30.724	62.832	1.00 46.63		С
	ATOM	15197		VAL C 201		31.231	31.274	61.575	1.00 46.72		C.
25	ATOM			VAL C 201		32.720	31.290	61.826	1.00 46.42		C.
-25	MOTA	15199 15203		VAL C 201		30.925	30.490	60.319	1.00 43.26		C .
	MOTA	15203		VAL C 201		28.940	30.649	62.528	1.00 44.99		С
	MOTA			VAL C 201		28.376	29.572	62.414	1.00 54.23		0
	MOTA	15208	O N	ILE C 202		28.293	31.822	62.411	1.00 48.31		N
20	MOTA	15209	CA	ILE C 202		26.856	31.919	62.056	1.00 42.18		С
30	MOTA	15211 15213	CB	ILE C 202		25.960	32.584	63.153	1.00 46.13		C
	ATOM			ILE C 202		25.705	31.620	64.319	1.00 52.03		С
	MOTA	15215		ILE C 202		25.448	32.297	65.708	1.00 47.21		С
	MOTA	15218		ILE C 202		24.579	32.776	62.594	1.00 47.93		С
25	ATOM	15222	C	ILE C 202		26.593	32.612	60.710	1.00 43.46		C
35	MOTA	15226	0 .	ILE C 202		26.878	33.802	60.543	1.00 38.75		o
	MOTA	15227		ILE C 202		26.020	31.835	59.782	1.00 42.36		N.
	ATOM	15228 15230	N CA	ILE C 203		25.653	32.266	58.452	1.00 38.42		С
	MOTA	15232	CB	ILE C 203		25.821	31.121	57.521	1.00 39.19		С
40	ATOM	15234		ILE C 203		27.291	30.844	57.270			С
40	ATOM ATOM	15237		ILE C 203		27.493	29.632	56.433	1.00 33.12		С
	ATOM	15241		ILE C 203		25.129	31.425	56.216	1.00 43.76		С
	MOTA	15241	C	ILE C 203		24.172	32.651	58.419	1.00 46.84		C
	ATOM	15246	.0	ILE C 203		23.325		58.599	1.00 42.94		Ò
45	ATOM	15247	N	VAL C 204		23.882	33.938	58.150	1.00 44.19		N
. TJ	ATOM	15249	CA	VAL C 204		22.544	34.494	58.261	1.00 40.88		С
	ATOM	15251	CB	VAL C 204		22.551	35.857	58.956	1.00 39.68		С
	ATOM	15253		VAL C 204			35.782		1.00 45.63		С
	ATOM	15257		VAL C 204		23.163	36.889	58.094	1.00 38.86		С
50	ATOM	15261	C,	VAL C 204		21.836	34.673	56.947	1.00 41.55		С
50		15262	ŏ	VAL C 204		20.631	34.867	56.901	1.00 40.27		О
	MOTA	15263	N	ARG C 205		22.546	34.630	55.851	1.00 44.70		N
	MOTA	15265	CA	ARG C 205		21.813	34.671	54.594	1.00 43.15		·C
	MOTA	15267	CB	ARG C 205		21.363	36.095	54.387	1.00 42.20		C
55	ATOM		CG	ARG C 205	•	20.722	36.355	53.055	1.00 45.65		C
55	ATOM	15270	CD	ARG C 205		20.529	37.833	52.808	1.00 40.86		С
	MOTA	15273	NE	ARG C 205		20.356		51.406			N
	ATOM	15276	CZ	ARG C 205		19.209	38.492	50.860			С
	ATOM	15278		ARG C 205		18.138	38.663	51.623			N
60	ATOM	15279		ARG C 205		19.131	38.724	49.538			N
UU	ATOM	15282		ARG C 205		22.634	34.130	53.409			Ċ
	MOTA	15285	.0	###G C 203		22.037	3.0.200				

									1 00	41 00			0
5	MOTA	15286	Ο.	ARG C. 205		23.813	34.449	53.284		41.99			
•	MOTA	15287	·N	VAL C 206		22.026	33.317	52.550		40.52			N
	ATOM	15289	CA	VAL C 206		22.737	32.791	51.379		41.02			C
	ATOM	15291	CB	VAL C 206		22.927	31.279	51.471		40.59			С
	ATOM	15293		VAL C 206		23.317	30.696	50.129		42.15			. C
10	ATOM	15297		VAL C 206		24.031	30.961	52.462	1.00	41.87			С
10	ATOM	15301	C	VAL C 206		22.034	33.153	50.075	1.00	43.12			С
			0	VAL C 206		20.813	33.046	49.996		47.55			0
	MOTA	15302		GLU C 207		22.806		49.065		44.82			N
	ATOM	15303	N	GLU C 207		22.279	34.018	47.753		41.44			С
	MOTA	15305	CA				35.512	47.568		41.47	•		С
.15	MOTA	15307	CB	GLU C 207	٠.	22.430		48.314		42.60			C.
	ATOM	15310	CG	GLU C 207		21.512	36.430			50.19			C
	ATOM	15313	CD	GLU C 207		22.035	37.856	48.249		52.39			o.
•	MOTA	15314		GLU C 207		22.821	38.160	47.296					ŏ
	ATOM	15315	OE2	GLU C 207		21.679		49.147		46.64			c
20	MOTA	15316	С	GLU C 207		23.034	33.399	46.566		41.75			
	MOTA	15317	0	GLU C 207		24.211	33.080	46.689		36.68			0
	ATOM	15318	N	ILE C 208		22.342	33.253	45.423		40.80			N
	ATOM	15320	CA	ILE C 208		22.905	32.702	44.200		40.34	•	•	С
	ATOM	15322	СВ	ILE C 208		22.245	31.408	43.864		39.20	•		С
25	ATOM	15324		ILE C 208		22.071	30.557	45.096		40.09			С
29	ATOM	15327		ILE C 208		23.285	29.762	45.470	1.00	40.99		•	C
	ATOM	15331		ILE C 208		23.075	30.663	42.809	1.00	43.38			С
			C	ILE C 208			33.697	43.111		42.32			C.
	ATOM	15335		ILE C 208			33.839	42.734		52.77	•		0
20	MOTA	15336	0			23.622	34.358	42.581		46.89		•	N
.30	ATOM	15337	N.	ASN C 209		23.490	35.589	41.739		39.83			С
	ATOM	15339	CA	ASN C 209			35.302	40.256		34.52			C
	ATOM	15341	CB-	ASN C 209		23.200		39.447		36.76			Č
	ATOM	15344	CG	ASN C 209		24.501	35.018			41.74			ŏ
	ATOM	15345		ASN C 209		25.573	35.001	40.006		39.00			N
35	ATOM	15346		ASN C 209	•	24.391		38.132		37.58			C
	MOTA	15349	С	ASN C 209		22.527	36.598						Ö
	MOTA	15350	0	ASN C 209		21.701	37.132	41.701		48.40			N
•	MOTA	15351	N	GLY C 210		22.673	36.854	43.652		46.50			C
	ATOM	15353	CA	GLY C.210		21.882	37.848	44.370		41.31			
40	ATOM	15356	С	GLY C 210		20.518	37.398	44.884		41.24			C
	MOTA	15357	0	GLY C 210		19.844	38.161	45.549		37.25			0
	ATOM	15358	N	GLN C 211		20.113	36.163	44.594		46.35			N
	MOTA	15360	CA	GLN C 211		18.781	35.675	44.963		45.47	•		C
	ATOM	15362	CB	GLN C 211		18.262	34.732	43.882		49.01			C
45	ATOM	15365	CG	GLN C 211		16.792	34.340	44.050		48.53			С
	ATOM	15368	CD	GLN C 211		16.314	33.366	42.969	1.00	52.21			С
	ATOM	15369		GLN C 211		17.113	32.799	42.237		59.52			. 0
	ATOM	15370	NE2	GLN C 211	•	15.007	33.168	42.882	1.00	62.94			N
	ATOM	15373	C	GLN C 211		18.784	34.920	46.237	1.00	44.55			C
-50	ATOM	15374	ō	GLN C 211		19.593		46.396	1.00	47.96			0
30		15375	N .	ASP C 212		17.866	35,263	47.137		47.82			N
	ATOM			ASP C 212		17.721	34.610	48.445		48.03		•	С
	ATOM	15377	CA	ASP C 212		16.568		49.184		46.60			, C
	ATOM	15379	CB				•	50.710		54.20			C
	ATOM		CG	ASP C 212		16.680		51.273		61.39			ō
55	MOTA			ASP C 212		17.374	34.336						ŏ
	ATOM			2 ASP C 212		16.077		51.457		0 60.59			c
	MOTA			ASP C 212		17.410		48.296		52.45		•	Ö
	ATOM	15386	0	ASP C 212		16.578		47.490		56.67			
	MOTA	15387	N	LEU C 213		18.087		49.055		55.42			N
60	ATOM		CA	LEU C 213		17.742				56.97			Ç
		·15391		LEU C 213		18.895	30.033	49.754	1.00	58.95			C
													•

5	ATOM	15394	CG	LEU C 213		19.416	28.788	49.047		59.16				C
,	ATOM	15396		LEU C 213		20.101	29.126	47.742		63.01				C
	ATOM	15400		LEU C 213		20.399	28.127	49.943		60.50				С
	ATOM	15404	С	LEU C 213		16.458	30.806	50.017	1.00	62.07				С
	ATOM	15405	ō	LEU C 213		15.551	29.957	49.888	1.00	61.04				0
10	ATOM	15406	N	LYS C 214		16.396	31.769	50.929	1.00	63.07				N
10	ATOM	15408	CA	LYS C 214		15.125	32.134	51.531	1.00	65.72				С
	ATOM	15410	CB	LYS C 214		14.086	32.338	50.413	1.00	68.54				C
	ATOM	15413	CG	LYS C 214		13.163	33.531	50.668	1.00	73.60				С
	ATOM	15416.	CD	LYS C 214		11.780	33.375	50.049	1.00	77.37				С
15	ATOM	15419	CE	LYS C 214		10.778	34.279	50.782	1:00	80.25				С
15		15422	NZ	LYS C 214		9.511	34.543	49.997	1.00	81.27			•	N ·
	MOTA	15426	C	LYS C 214		14.595	31.119	52.502		65.65				С
	ATOM	15427	Ö	LYS C 214	•	13.379	30.934	52.638	1.00	66.01.				0
٠.	ATOM	15427	N	MET C 215		15.509	30.463	53.188		63.58	•			N
20	MOTA	15430	CA	MET C 215		15.135	29.471	54.158		61.94				C
20	ATOM		CB	MET C 215		16.070		53.990		61.98	•			C
	MOTA	15432	CG	MET C 215		15.962	27.721	52.571		65.30				С
	MOTA	15435		MET C 215		17.057	26.390			66.94				S
	ATOM	15438	SD			17.630	26.053	53.654		69.99				С,
0.5	ATOM	15439	CE	MET C 215 MET C 215		15.206	30.067	55.558		61.53				C
25	MOTA	15443	C			15.628	31.208	55.733		62.98				0
	MOTA	15444	0	MET C 215 ASP C 216		14.770	29.312	56.552		59.98	•			N
	MOTA	15445	N	ASP C 216		14.984	29.732	57.917		63.83				C
	ATOM	15447	CA			14.421	28.723	58.910		63.59				C
20	MOTA	15449	CB	ASP C 216		14.421	29.219	60.341		63.16				C
30	ATOM	15452	CG	ASP C 216		15.548	29.759	60.739		69.24				Ō
	ATOM	15453		ASP C 216		13.541	29.119			58.32				0
	ATOM	15454		ASP C 216		16.489	29.813	58.110		67.41				С
	MOTA	15455	С	ASP C 216		17.241	28.950	57.662		70.90				Ō
	ATOM	15456	0	ASP C 216		16.938	30.845	58.787		68.15				N
35	ATOM	15457	N	CYS C 217		18.351	31.024	58.969		72.70		٠		C
•	MOTA	15459	CA	CYS C 217		18.529	32.328	59.712		74.24				C
	MOTA	15461	CB	CYS C 217		18.246	32.242	61.449		86.77				5
•	ATOM	15464	SG	CYS C 217 CYS C 217		19.059	29.819	59.668		71.10				C
40	MOTA	15465	C	CYS C 217		20.134	29.351	59.235		66.77			•	Ō
40	MOTA	15466	0		,	18.447	29.314	60.736		70.12		•		N.
	ATOM	15467	N	LYS C 218		18.971	28.156	61.466		67.64				C
	ATOM	15469	CA			17.922	27.688	62.483		67.20		٠		C
	ATOM	15471	CB	LYS C 218		17.853	28.475	63.795		70.89				С
15	ATOM	15474	CG	LYS C 218		17.000	27.722	64.838		73.15				C
45	MOTA	15477	CD	LYS C 218 LYS C 218		16.593	28.602			74.74				С
	ATOM	15480	CE			15.949	29.917	65.624	•	73.64				N
	MOTA	15483	NZ	LYS C 218		19.318				63.47				C
	ATOM	15487	С	LYS C 218			26.234	60.716		60.95				ō
~0	ATOM	15488	0	LYS C 218		20.271	26.865	59.462		60.07				N
50	ATOM	15489	N	GLU C 219		18.540		58.582		60.47				C
	ATOM	15491	CA	GLU C 219		18.752	25.751	57.552		61.66			•	Č
	ATOM	15493	CB	GLU C 219		17.606		57.549		68.73				C.
	ATOM	15496	CG	GLU C 219		16.924	24.226			79.28			•	č
	ATOM		CD	GLU C 219		15.776		58.574						ŏ
55	ATOM			L GLU C 219		14.678		58.418		80.66				ő
	MOTA			2 GLU C 219.		15.962		59.549		81.82				·C
•	MOTA			GLU C 219		20.130				56.72 59.58				ő
	ATOM			GLU C 219		20.748								N
	MOTA		N	TYR C 220		20.643				56.94				C
60	MOTA			TYR C 220		22.003				51.25 50.12	. •			·C
	MOTA	15508	CB	TYR C 220		22.231	28.803	56.908	1.00	JU.12				•

5	ATOM	15511	CG	TYR C	220.	21.253	29.350	55.891	1.00 51.08		С
,	ATOM	15512		TYR C		20.657	30.589	56.072	1.00 52.25		C.
	ATOM	15514		TYR C		19.758	31.101	55.142	1.00 50.67		C
	ATOM	15514	CZ	TYR C		19.460	30.362	54.028	1.00 48.80		Ċ
	ATOM	15517	OH	TYR C		18.584	30.861	53.123	1.00 54.70		0
10	ATOM	15519		TYR C		20.029	29.140	53.811	1.00 47.32		Ċ
10	ATOM	15521		TYR C		20.927	28.634	54.741	1.00 53.35		Ċ
	ATOM	15523	C	TYR C		23.106	26.890	58.295	1.00 50.69		Č
	ATOM	15524	0	TYR C		24.252	26.689	57.913	1.00 49.00		Ŏ.
		15525	Ŋ	ASN C		22.780	26.754	59.569	1.00 50.57		N
15	MOTA	15527	CA	ASN C		23.770	26.262	60.506	1.00 55.15		Ċ
13	ATOM	15527	CB	ASN C		24.208	27.421	61.384	1.00 55.72		č
·	ATOM		CG	ASN C		24.244	28.687	60.624	1.00 58.30		č
	ATOM-	15532 15533		ASN C		25.274	29.062	60.045	1.00 61.72		ō
•	ATOM			ASN C		23.104	29.357	60.582	1.00 60.35	•	N
άn	ATOM	15534				23.219	25.081	61.310	1.00 55.63		C
20	ATOM		, C	ASN C		23.444	24.978	62.517	1.00 53.03		ŏ
	ATOM	15538	0	ASN C		22.510	24.378	60.627	1.00 55.35		N
	ATOM	15539	N	TYR C			23.173	61.334	1.00 55.70	•	Ç
	MOTA	15541	CA	TYR C		21.764	22.579	60.521	1.00 59.55		Ċ.
26	ATOM	15543	CB	TYR C		20.643		61.212	1.00 63.51	•	C
25	ATOM	15546	CG	TYR C		20.139	21.358 21.375	62.578	1.00 65.98		c
	ATOM	15547		TYR C		19.875		63.230	1.00 69.85		Ċ
	ATOM	15549		TYR C		19.414	20.235		1.00 72.74		C
	MOTA	15551	CZ	TYR C		19.215	19.049 17.898	62.511	1.00 72.74		o
20	ATOM	15552	OH	TYR C		18.757		63.130	1.00 71.88		C
30	ATOM	15554	CE2			19.476	19.019	61.155	1.00 72.46		C
	ATOM	15556		TYR C		19.940	20.174	60.515			. C
	ATOM	15558	С	TYR C		22.748	22.140	61.714	1.00 55.15 1.00 51.38		0
		15559	0	TYR C		23.304	21.468	60.853 63.027	1.00 51.38		N
25	MOTA	15560	N	ASP C		22.904	22.013 21.398	63.668	1.00 57.35		C
35	ATOM	15562	CA	ASP C		24.044	20.222	62.885	1.00 64.20		C
	MOTA	15564	CB	ASP C		24.600 25.633	19.430	63.682	1.00 68.05		Č
	ATOM	15567	CG OD1	ASP C		26.491	18.782	63.058	1.00 05.03		Ö
	MOTA	15568		ASP C		25.669	19.410	64.935	1.00 65.90		Ö
40	MOTA	15569		ASP C		25.109		63.857	1.00 53.89		Ċ
. 40	MOTA	15570	С 0	ASP C		25.364	22.902	64.969	1.00 51.49		ő
	ATOM ATOM	15571 15572	•	LYS C		25.729	22.980	62.788	1.00 51.45		N
	ATOM	15574	N CA	LYS C		26.750	24.020	62.949	1.00 48.28		C
	MOTA	15576	CB	LYS C		27.919	23.538	63.825	1.00 49.33		Č
45	ATOM	15579	CG	LYS C		28.786	22.456	63.125	1.00 50.13		č
	ATOM	15582	CD	LYS C		29.770	21.673	64.049	1.00 51.00		č
٠.	MOTA		CE	LYS C		29.958	20.230	63.586	1.00 56.39		· č
		15588	NZ	LYS C			19.360	63.812	1.00 54.03		N
			C.	LYS C		27.355	24.489	61.644	1.00 50.04		c
50	MOTA	15592		LYS C		27.279	23.799	60.619	1.00 30.04		ő
50	ATOM	15593	0 N	SER C		27.960	25.684	61.708	1.00 50.25		N
	ATOM	15594	N	SER C		28.747	26.210	60.604	1.00 30.23		C
	ATOM	15596	CA	SER C			27.468	60.076	1.00 47.14	•	c
	ATOM	15598	CB			28.098	27.124	59.460	1.00 47.14		o
55	ATOM	15601	OG C	SER C		26.865					c
55	ATOM	15603	C	SER C		30.179	26.415	61.102	1.00 44.94		0
	ATOM	15604	O N	SER C		30.396	27.152	62.055 60.479			N
	ATOM	15605	N	ILE C		31.149	25.745	60.888	1.00 45.19		C
	MOTA	15607	CA	ILE C		32.557	25.868 24.557	61.593	1.00 43.93		C
60	ATOM	15609	CB CG1	ILE C		33.045	24.557	60.579	1.00 39.91 1.00 39.64		C
UU	ATOM	15611		ILE C		33.415	23.500 22.226	61.231	1.00 39.64		C
	ATOM	15614	, UI	ILE C	. 220	34.031	22.220	4.634	1.00 37.70		J

5	ATOM	15618	CG2	ILE C	226	31.999		62.556		42.23			С
	ATOM	15622	С	ILE C	226	33.472				43.36			С
	MOTA	15623		ILE C		33.060		58.545		42.72	-		0
	ATOM	15624		VAL C		34.717		60.020		45.45			N
	ATOM	15626		VAL C		35.743		59.000		48.25			C
10	ATOM	15628		VAL C		36.309		59.169		47.46			C
	ATOM	15630		VAL C		37.483		58.234		46.44			C
	ATOM	15634	CG2	VAL C	227	35.243		58.940		48.83			C
	MOTA	. 15638		VAL C		36.907				44.62			С
٠.	MOTA	15639		VAL C		37.588		60.143		41.47			0
15	ATOM	15640		ASP C		37.146		58.043		45.60			N C
	MOTA	15642		ASP C			3 24.013	58.065		43.43			Ç.
	ATOM	15644		ASP C		37.293				44.61 49.06	·		c .
	MOTA	15647		ASP C		38.162		58.399		51.29			0
	MOTA	15648		ASP C		39.34		58.748		48.80			0
20	MOTA	15649			228		•	58.225					c
	MOTA	15650	C.	ASP C		39.05		56.868		42.97			0
	ATOM	15651		ASP C		38.66		55.830		51.06 42.95			N
	MOTA	15652	N	SER C		40.31		57.035					C
	ATOM	15654	CA	SER C		41.35		55.999		42.72 45.39			c
25	MOTA	15656	CB	SER C		42.64	•	56.493		48.69			Ö
	ATOM	15659	OG	SER C		43.16		57.661		43.75			c
	MOTA	15661	С	SER C		41.71	•	55.619 54.667		44.82			Ö
	ATOM	15662	0		229	42.44		56.389		47.33			N
20	MOTA	15663	N	GLY (41.25	-	56.072		45.82			c
30	MOTA	15665	CA	GLY (41.47 40.32		55.294		47.37			c
	ATOM	15668	C		230	40.32		55.074		50.08			o
	MOTA	15669	0		230	39.32		54.875		50.13			N
	ATOM	15670	N		231	38.12		54.126		44.81			C
35	MOTA	15672 15674	CA CB		231	36.84		54.846		41.41			C
33	ATOM ATOM	15676		THR (36.87		56.171		42.47			0
	ATOM	15678		THR (35.73		54.262		45.87			C
	ATOM	15682	C		231	38.09		52.773		46.97			C
	ATOM	15683	Ö		C 231	38.22		52.653		41.58			0
40	ATOM	15684	N		232	37.90		51.755	1.00	47.97			N
	ATOM	15686	CA		C 232	38.11		50.382	1.00	48.47			С
	ATOM	15688	СВ		C 232	38.31		49.509	1.00	47.83			С
	ATOM	15690			C 232	39.51		49.871	1.00	46.26			0
	ATOM	15692			C 232	38.58		48.087	1.00	52.26			C
45	ATOM	15696	C		C 232	36.99	1 21.136	49.741	1.00	49.88			С
	ATOM	15697	0		C 232	37.26		48.965	1.00	52.26		•	0
	ATOM	15698	N		C 233	35.74	3 20.788	50.054		47.73		•	N
	ATOM	15700	CA	ASN	C 233	34.58	6 21.318	49.385	1.00	44.90			С
	ATOM	15702	СВ		C 233	33.57			1.00	44.37			Ċ.
50	ATOM	15705	CG		C 233	34.02	5 19.181	48.006		47.43			С
	MOTA	15706	OD1	ASN	C 233	35.05	19.285	47.345	1.00	52.27			0
	ATOM	15707			C 233	33.21	6 18.155	47.871	1.00	47.91			N
	ATOM	15710	С		C 233	33.86	55 - 22.287	50.313		49.52			С
	MOTA	15711	0	ASN	C 233	34.28	33 22.502	51.451	1.00	51.70			0
55	MOTA	15712	N	LEU	C 234	32.78	37 22.878			49.50			N
	ATOM	15714	CA	LEU	C 234	31.85				50.43			С
	MOTA	. 15716	CB	LEU	C 234	31.16				49.25			C
	MOTA	15719	CG		C 234	30.57				46.33			C
	ATOM	15721			C 234	29.47				40.51			C
60	MOTA	15725	CD2		C 234.	30.09				46.97			C
	MOTA	15729	C ·	LEU	C 234	30.85	52 22,593	50.965	1.00	49.62			С

•	2004	16720	•	LEU C 23	2.4	30.407	21.816	50.116	1.00	45.22		0
5	MOTA	15730	0	ARG C 23		30.491	22.520	52.239		48.90		N
	ATOM	15731	N			29.625	21.424	52.677		44.81		С
	ATOM	15733	CA	ARG C 23		30.348	20.503	53.656		43.27		С
	MOTA	15735	CB	ARG C 23		31.341	19.584	53.002		43.89		C
	MOTA	15738	CG	ARG C 23			18.160	52.801		50.43		С
10	ATOM	15741	CD	ARG C 2		30.842		53.837		50.04		N
	MOTA	15744	NE	ARG C 2		31:337	17.255			45.48		c
	MOTA	15746	CZ	ARG C 2		31.221	15.938	53.811		46.80		N
	ATOM	15747		ARG C 2		31.708	15.258	54.800		47.49		N
	ATOM	15750	NH2	ARG C 2		30.623	15.297	52.831		40.98		C
15	MOTA	15753	С	ARG C 2		28.396	21.986	53.309				0
	ATOM	15754	0	ARG C 2		28.468	22.809	54.227		37.83		N
	ATOM	15755	N	LEU C 2	36	27.250	21.535	52.823		39.74		
	ATOM	15757	CA	LEU C 2	36	26.029	22.121	53.291		40.54		C
	ATOM	15759	CB	LEU C 2	36	25.356	23.023	52.230		44.87		C
20	ATOM	15762	CG	LEU C 2	36	26.128	24.202	51.585		44.63		С
	ATOM	15764	CD1	LEU C 2	36	26.000	24.076	50.073		44.76		С
	ATOM	15768		LEU C 2		25.626	25.572	52.036		45.65		С
	MOTA	15772	С	LEU C 2		25.108	21.049	53.643	1.00	43.06		Ç
	ATOM	15773	Ō.	LEU C 2		24.992	20.025	52.998	1.00	50.00		0
25	ATOM	15774	N	PRO C 2		24.421	21.296	54.709	1.00	43.05		N
23	ATOM	15775	CA	PRO C 2		23.369	20.404	55.125	1.00	47.30		С
		15777	CB	PRO C 2		22.620	21.271	56.095	1.00	43.42		С
	ATOM		CG	PRO C 2		23.724	22.119	56.697		39.72		C
	ATOM	15780				24.594	22.448	55.598		39.54		С
ań	MOTA	15783		PRO C 2		22.468	19.981	53.957		56.07		C
30	ATOM	15786	C	PRO C 2		22.182	20.767	53.053		61.19		0
	ATOM	15787	0				18.724	54.011		64.48		N
	MOTA	15788	N	LYS C 2		21.060	18.088	53.117		67.74		C
	MOTA	15790	CA	LYS C 2			16.981	53.939		70.89		С
	MOTA	15792	CB	LYS C 2		20.344	16.043	53.183		75.72		c
35	MOTA	15795	CG	LYS C 2		19.364		52.057		77.64		C
	MOTA	15798	CD	LYS C 2		20.022	15.198	51.786		76.46		c
	MOTA	15801	CE	LYS C 2		19.238	13.898			74.66		N
	MOTA	15804	NZ	LYS C 2		19.681	13.117	50.588		67.39		C
Α.	MOTA	15808	С	LYS C 2		20.005	19.015	52.472		67.71		ŏ
40	MOTA	15809	0	LYS.C 2		19.814	19.005	51.247				N
•	MOTA	15810	N	LYS C 2		19.303	19.801			64.13		Ċ
	MOTA	15812	CA	LYS C 2		18.305	20.683	52.716		64.27		C
	ATOM	15814	CB	LYS C 2		17.338	21.171	53.792		68.69		C
	ATOM	15817	CG	LYS C 2		16.086	20.292	53.968		74.28		C
45	MOTA	15820	CD	LYS C 2		15.063	20.977	54.894		76.92		
	MOTA	15823	CE	LYS C 2		14.640	22.366	54.381		76.03		C
	ATOM	15826	NZ	LYS C 2	239	13.915	23.177	55.415		74.75		N
	ATOM	15830	С	LYS C 2	239	18.918	21.886	52.013		62.66		C
•	ATOM	15831	0	LYS C		18.495	22.234	50.903		62.29		0
50	ATOM	15832	N	VAL C		19.913	22.528	52.637		56.54		N
	ATOM	15834	CA	VAL C		20.450	23.737	52.039		48.20		C
	ATOM	15836	CB	VAL C		21.459	24.457	52.876	1.00	47.96		С
	ATOM	15838		L VAL C		21.799	25.770	52.198	1.00	51.82		C
	ATOM	15842		2 VAL C		20.934	24.744	54.268	1.00	49.07		С
55				VAL C		21.110	23.315	50.780		44.11		С
JJ	MOTA		Ö	VAL C		21.003	23.955	49.756		40.57		0
	MOTA			PHE C		21.797	22.200			43.45		N
	MOTA			PHE C		22.457	21.728	49.645		44.85		С
	ATOM					23.107				44.07		C
C 0	ATOM					23.738		48.699	•	0 44.31		c
60	MOTA					25.736				0 40.53		Č
	ATOM	15856	CD	1 PHE C	241	25.015	20.034	40.509	.2.01			_

		.					•						
5	ATOM .	15858	CE1	PHE C 2	241	25.575	19.460	47.272	1.00	42.85			С
_	ATOM	15860	CZ	PHE C 2		24.879	18.608	46.499	1.00	35.50			С
	MOTA	15862	CE2	PHE C 2	241	23.628	18.323	46.804	1.00	37.83			С
	ATOM	15864	CD2	PHE C 2	241	23.039	18.897	47.899	1.00	44.17			С
	ATOM	15866	С	PHE C 2	241	21.495	21.587	48.488	1.00	46.73			C
10	ATOM	15867	ο.	PHE C 2	241	21.880	21.762	47.328	1.00	46.03			Ö
10	ATOM	15868	N	GLU C 2		20.241	21.294	48.824	1.00	50.74			N
	ATOM	15870	CA	GLU C 2		19.228	20.899	47.851	1.00	51.33			С
	ATOM	15872	CB	GLU C 2		18.100	20.168	48.570	1.00	56.02			С
	ATOM	15875	CG	GLU C 2		18.214	18.657	48.515	1.00	62.01			C
15	ATOM	15878	CD	GLU C 2		18.576	18.183	47.122	1.00	66.03	•		С
••	ATOM	15879		GLU C 2		18.159	18.881	46.155	1.00	67.53			0
	ATOM	15880		GLU C 2		19.277	17.134	46.997	1.00	60.97			0
	ATOM	15881		GLU C 2		18.645	22.076	47.116	1.00	50.90			С
•	ATOM	15882	Ō	GLU C 2		18.470	22.057	45.901	1.00	46.64			0
20	ATOM	15883	N	ALA C 2		18.337	23.100	47.883	1.00	47.93			N
20	ATOM	15885	ĊA	ALA C 2		17.831	24.310	47.324	1.00	50.32			C
•	ATOM	15887	СВ	ALA C 2		17.431	25.228	48.429		49.97			С
	ATOM	15891	C.	ALA C 2		18.932	24.932	46.484	1.00	53.72			C
	ATOM	15892	0	ALA C 2		18.694	25.406	45.376	1.00	58.27			0
25	ATOM	15893	N	ALA C 2		20.142	24.925	47.020	1.00	55.49			N
	ATOM	15895	CA	ALA C 2		21.270	25.524	46.335	1.00	53.08			С
	ATOM	15897	CB	ALA C 2		22.505	25.573	47.229	1.00	55.11			Ç
	ATOM	15901	C	ALA C 2		21.575	24.821	45.057	1.00	53.02			С
	ATOM	15902	Ō	ALA C 2		21.779	25.481	44.073		60.49			0
30	ATOM	15903	N	VAL C 2		21.608	23.495	45.025	1.00	56.92			N
	ATOM	15905	CA	VAL C 2		21.907	22.825	43.748	1.00	53.60			C
	ATOM	15907	СВ	VAL C 2		22.025	21.300	43.842	1.00	55.63		•	С
	ATOM	15909		VAL C 2		22.667	20.709	42.554	1.00	54.38			С
•	ATOM	15913		VAL C 2		22.819	20.900	45.014	1.00	58.96			C
35	ATOM	15917	C	VAL C 2		20.804	23.069	42.734	1.00	55.12			c c
	ATOM	15918	0	VAL C 2	245	21.060	22.974	41.544	1.00	58.24			0
	ATOM	15919	N	LYS C 2		19.574	23.356	43.160	1.00	52.47			N
	ATOM	15921	CA	LYS C 2	246	18.549	23.620	42.157	1.00	58.91			С
	ATOM	15923	СВ	LYS C 2	246	17.129	23.817	42.754	1.00	62.86			C.
40	ATOM	15926	CG	LYS C 2	246	16.324	22.600	43.183	1.00	70.41			С
	ATOM	15929	CD	LYS C 2	246	16.388	21.363	42.223	1.00	76.82			С
	ATOM	15932	CE	LYS C 2	246	17.595	20.433	42.499		77.01			С
	ATOM	15935	NZ	LYS C 2	246	17.683	19.311	41.510	1.00	75.94			N
	ATOM	15939	C	LYS C 2	246	18.944	24.940	41.486		56.47			С
45	MOTA	15940	0	LYS C 2	246	19.066	25.062	40.257		59.03			0
	ATOM	15941	, N	SER C 2	247 .	19.153	25.920	42.348		47.24			N
	ATOM	15943	CA	SER C 2		19.348	27.272	41.934		47.24			C .
	ATOM	15945	CB	SER C 2		19.509	28.132	43.169		47.72			С
	ATOM	15948	OG	SER C 2		19.430	29.494	42.810		53.48			0
50	ATOM	15950	С	SER C 2	247	20.563	27.421	41.042		47.61			С
	MOTA	15951	0	SER C 2	247	20.552	28.143	40.030		48.26			, O
	ATOM	15952	N	ILE C 2	248	21.612	26.730	41.432		40.55			N
	ATOM	15954	, CA	ILE C.2	248	22.802	26.795	40.710		39.34		•	С
	ATOM	15956	CB	ILE C 2	248	23.804	25.942	41.355		39.28			С
55	ATOM	15958	CG1	ILE C 2	248	24.164	26.530	42.675	1.00	37.69			С
	MOTA	15961	CD1	ILE C 2	248	25.595	26.384	42.926	1.00	40.41			С
	ATOM	15965	CG2	ILE C 2		25.073	25.940	40.565		45.18			С
	ATOM	15969	С	ILE C 2	248	22.498	26.311	39.348		47.60			С
	MOTA	15970	0	ILE C 2		22.793	27.013	38.398		52.36			0
60	MOTA	15971	N	LYS C 2	249	21.894	25.118	39.244	•	54.81			N
	MOTA	15973	CA	LYS C 2	249	21,619	24.488	37.939	1.00	52.55			С

		•											_
5	ATOM	15975	СВ	LYS C 249	2				1.00				C :
J	ATOM		CG	LYS C 249	2	21.397	21.980		1.00				Ċ
	ATOM		CD	LYS C 249	2	20.426	20.783		1.00				c
	ATOM			LYS C 249		20.792	19.557			67.61			N
				LYS C 249	1	19.732	19.211	40.190	1.00	73.03			C
10	MOTA		C	LYS C 249	2	20.837	25.463	37.110	1.00	51.86			0
10	MOTA		ŏ	LYS C 249		21.209	25.796	35.990	1.00	56.70			N
	MOTA		N	ALA C 250		19.737	25.924	37.683		44.72			C
	MOTA	15995	CA	ALA C 250		18.871	26.855	36.999	1.00	43.29		٠	
	MOTA	15997	CB	ALA C 250		17.850	27.442	37.977		38.29			C
16	MOTA	16001	C	ALA C 250		19.696.	27.950	36.371		45.27			C
15	MOTA	16002	0	ALA C 250		19.535	28.253	35.199	1.00	46.37			0
	ATOM		N	ALA C 251		20.600	28.539	37.153	1.00	44.64		,	N
	ATOM	16005	CA	ALA C 251		21.362	29.667	36.658	1.00	42.02			C
	MOTA	16007	CB	ALA C 251		22.173	30.242	37.739	1.00	39.56			· C
	ATOM		CD	ALA C 251		22.237	29.272	35.492	1.00	44.55			C
20	MOTA	16011	0	ALA C 251		22.459	30.029	34.574		53.96			0
	ATOM	16012	N	SER C 252		22.716	28.059	35.523		48.25			.N
	MOTA	16013		SER C 252		23.581	27.567	34.487	1.00	50.72			C
	MOTA	16015	CA	SER C 252		24.561	26.537	35.095		50.46			С
	MOTA	16017	CB	SER C 252		24.087	26.053	36.372	1.00	50.66			0 ·
25	MOTA	16020	og C	SER C 252		22.746	26.890	33.427	1.00	51.45			C.
	MOTA	16022	С	SER C 252		23.305	26.186	32.595	1.00	54.49			0
	MOTA	16023	0	SER C 252		21.428	27.104	33.448	1.00	52.44			N
	ATOM	16024	N	SER C 253		20.502	26.337	32.588	1.00	55.69			С
	MOTA	16026	CA	SER C 253		19.025	26.589	32.995	1.00	58.26			С
30	MOTA	16028	CB	SER C 253		18.469	27.826	32.540		55.32			. 0
	MOTA	16031	QG C	SER C 253		20.673	26.458	31.073		58.55			С
	MOTA	16033	С	SER C 253		19.693	26.428	30.343		67.47			0
	MOTA	16034	0	THR C 254		21.917	26.600	30.614	1.00	62.21			N
	MOTA	16035	N	THR C 254		22.258	26.667	29.181	1.00	64.73			C
35	MOTA	16037	CA	THR C 254		22.914	27.939	28.896		66.84			C
•	ATOM	16039	CB	THR C 254		24.215	27.899	29.500	1.00	71.03			0
	MOTA		CC1	2 THR C 254		22.183	29.063	29.569		72.72			C.
	MOTA			THR C 254		23.294	25.658	28.754		68.84			С
40	ATOM		C O	THR C 254		23.746		27.602	1.00	68.20			0_
40	ATOM		. И	GLU C 255		23.714	24.865	29.712		69.98			N
	ATOM					24.513	23.729	29.447		0 69.15°			C,
	ATOM		CA CB			25.990			1.0	0 69.01			C,
	ATOM		CG			26.765		28.627		0 73.89			C
45	ATOM		CD			28.135		28.412		0 80.19			C
45	ATOM			1 GLU C 255		28.259		28.391		0 77.88	•		. 0
	ATOM			2 GLU C 255	•	29.078	24.723	28.256	1.0	0 75.03			. 0
•	ATOM			GLU C 255		23.813		30.451	1.0	0. 68.56			C
	ATOM			GLU C 255		23.260			1.0	0 63.70			0
50	ATON			LYS C 256		23.797			1.0	0 69.73			N.
50						23.140			1.0	0 69.57			C
	ATO			000		21.875			-1.0	0 71.79			C
	ATO			056		20.817			1.0	0 73.04		•	C
•		4 16071				20.475			1.0	0 75.70			C
	ATO					19.06			1.0	0 74.59			C
55				056		18.582			_	0 76.39			И
	ATO					24.21				0 67.18			C
	ATO			LYS C 256		25.20			3 1.0	0 58.20			0
	ATO			LYS C 256		24.07				00 68.64			И
	ATO			PHE C 257		25.04				00 69.01			C
60				A PHE C 257		26.00			9 1.6	00 72.10			C
	ATO	м 16090	D CI	B PHE C 257		20.00	J _ 10.00	5 54.00					

WO 03/012089 PCT/GB02/03461

5	ATOM	16093	CG	PHE C	257	26.744	20.209	33.362	1.00			С
٠,	ATOM	16094	CD1	PHE C	257	26.419	21.522	33.680	1.00			С
	ATOM	16096	CE1	PHE C	257	27.086	22.590	33.094	1.00			С
	ATOM	16098	CZ	PHE C		28.091	22.354	32.180	1.00			С
	ATOM	16100		PHE C		28.431	21.043	31.849	1.00	72.57		С
10	ATOM	16102		PHE C		27.755	19.980	32.439	1.00			С
10	ATOM	16104	C	PHE C		24.335	17.131	33.647	1.00	69.41		С
	ATOM	16105	Ō	PHE C		23.173	17.187	34.100	1.00	68.36		0
	ATOM	16106	N	PRO C		25.041	16.022	33.594	1.00	68.72 .		N
	ATOM	16107	CA	PRO C		24.559	14.751	34.139	1.00	72.08		С
15	ATOM	16109	СВ	PRO C		25.649	13.798	33704	1.00	72.60		С
13	MOTA	16112	CG	PRO C		26.863	14.705	33.627	1.00	72.00		С
	MOTA	16115	CD	PRO C		26.363	15.901	32.963		68.28		С
	ATOM	16118	C	PRO C		24.507	14.757	35.662	1.00	74.57		С
•		16119	Ö	PRO C		25.438	15.317	36.245		75.66		0
.20	ATOM	16120	N	ASP C		23.479	14.151	36.272		75.85		N.
20	ATOM		CA	ASP C		23.355	14.015	37.747		77.50	•	C
	MOTA	16122	CB.	ASP. C		22.436	12.845	38.118		77.91		С
• •	MOTA	16124		ASP. C		20.964	13.134	37.904		80.16	•	С
	MOTA	16127	CG	ASP C		20.559	14.322	37.914		84.49		0
25	MOTA	16128		ASP C		20.138	12.206	37.727		74.07		o
25	MOTA	16129				24.649	13.750	38.543		77.00		C
	ATOM	16130	С	ASP C		24.727	14.079	39.732		79.56		ō
	ATOM	16131	0	ASP C		25.648	13.148	37.914		75.01		N
	MOTA	16132	N	GLY C		26.852	12.769	38.636		75.71		c
20	ATOM	16134	CA	GLY C		27.782	13.929	38.922		74.37		Č
30	MOTA	16137	C	GLY C		28.535	13.929	39.919		75.33		ō
	MOTA	16138	0	GLY C			14.918	38.035		69.34		N
	ATOM	16139	N	PHE C		27.730	16.095	38.171		62.53		c
	ATOM	16141	CA	PHE C		28.550	17.037	36.990		63.25		c
~-	MOTA	16143	CB	PHE C		28.341	18.334	37.098	•	57.93		č
35	ATOM	16146	CG	PHE C		29.079	18.360	37.184		55.84		č
	ATOM	16147		PHE C		30.455	19.557	37.104		55.60	•	·C
	ATOM	16149		PHE C		31.129	20.732	37.293		55.30		c
	ATOM	16151	CZ	PHE C		30.424 29.056	20.732	37.210		56.24		Č
40	ATOM	16153		PHE C			19.522	37.210		55.44		Č
40	ATOM	16155		PHE C		28.393 28.026	16.693	39.413		58.82		Č
	ATOM	16157	C	PHE C		28.717	16.758	40.395		61.51		o
	ATOM	16158	0.		261	26.772	17.095	39.384		58.00		N
	ATOM	16159	N	TRP C		26.179	17.725	40.536		59.65		c
45	ATOM	16161	CA	TRP C		24.722	18.071	40.271		64.16		č
45	ATOM	16163	CB	TRP C			19.084	39.179		67.86		C
	ATOM	16166		TRP C		24.498	18.900	38.046		69.53		Č
	ATOM	16167				23.762		37.278		70.01		N
	ATOM	16169	NE1			23.775	20.992	37.910		68.68		c
50	ATOM	16171		TRP C		24.527	20.427	39.113		67.00		c
50	MOTA	16172		TRP.C		24.995	21.210	39.941		69.48		c
	MOTA	16173		TRP C		25.793		39.547		69.43		c
	ATOM	16175		TRP C		26.091	22.516	38.351		66.24		Ċ
	MOTA	16177		TRP C		25.608	23.038			66.76		c
	ATOM	16179		TRP C		24.830	22.295					Č
55	ATOM	16181	C	TRP C		26.284	16.847	41.766 42.869		58.97 57.31		0
	MOTA		0	TRP C		26.059						N
	ATOM	16183	N	LEU C		26.601	15.574	41.597		65.06		C
	ATOM	16185	CA	LEU C		26.806		42.767		67.45		C
	MOTA	16187	CB	LEU (26.279		42.533		68.47		C
60	MOŢA	16190	CG	LEU (24.933		43.225		72.82		·C
	MOTA	16192	CD1	LEU (263	24.425	11.685	42.977	1.00	71.73		· C

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25.028 13.405 44.740 1.00 73.38
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                                                                                                          43.160
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                                           LEU C 263
                                                                         28.268
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                                    С
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                                                                         28.647
                                                                                          13.948
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                                                                                                          42.449
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                                           GLY · C 264
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                                                                                         15.429
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                                           GLY C 264
                                                                          30.488
                                                                                          15.522
                      16204
          MOTA
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                                                                                                         42.369 1.00 74.99
                                           GLY C 264 .
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                                                                                         14.276
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                                                                                                         42.728 1.00 77.68
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                                   0
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                                                                                         13.377
                                            GLU C 265
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                                   N
                                                                                         12.097
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                                                                          31.266
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                                                                          30.247
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          ATOM 16213
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                                                                                                          42.883
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                                                                                                                                                                     C
15
                     16216
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          MOTA
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28.455 9.405

28.654 8.812

31.978 12.017

32.902 11.222

31.566 12.831

32.162 12.771

31.280 12.063

29.788 12.214

29.003 11.021

28.246 10.351

29.191 10.748
                                                                                            9.514 43.067
                                                                                                                                                                     С
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                                           GLU C 265
          MOTA
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                                    OE1 GLU C 265
                                                                                                          44.208
                     16220
          ATOM
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                                                                                                          42.080
                                                                                                                          1.00 88.76
                                    OE2 GLU C 265
                     16221
          MOTA
                                                                                                                          1.00 73.02
                                                                                                          39.999
                                            GLU C 265
          MOTA
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                                    С
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                                                                                                                          1.00 73.00
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                                    CA
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                                                                                                                                                                     C
                                                                                                          36.972
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          MOTA
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25
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                                                                                                          37.140
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32.393 14.164 37.330
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                                                                                                          36.433
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                                            LEU C 267
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30
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                      16241
                                   N
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                                    ĊA
                                           LEU C 267
          MOTA
                                                                                                          36.200
                                                                                                                          1.00 66.35
                                            LEU C 267
                                                                          35.351
                                                                                          15.611
          ATOM 
                      16245
                                    CB
                                                                                                          35.211
                                                                                                                           1.00 65.47
                                                                          35.956
                                                                                          14.641
          MOTA
                      16248
                                    CG
                                            LEU C 267
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                                                                                                          33.871
                                                                                                                           1.00 70.86
                      16250
                                           LEU C 267
                                                                                          14.904
          ATOM
                                    CD1
                                                                                                                          1.00 67.21
                                    CD2 LEU C 267
                                                                          37.458
                                                                                          14.823
                                                                                                         35.131
35.
                      16254
          MOTA
                                                                                                                                                                     С
                                                                                                         34.883
                                                                                                                           1.00 66.62
                      16258
                                    С
                                            LEU C 267
                                                                         33.306 16.140
          MOTA
                                                                                                                           1.00 68.94
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                                            LEU C 267
                                                                         32.568
                                                                                          15.458
                                                                                                          34.196
                      16259
          ATOM
                                    0
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                   С
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           16598
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     ATOM 16599
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                       GLY C 289
     ATOM 16601
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29.552 41.029

28.759 40.561

30.527 41.828

30.713 42.194

32.131 42.676

33.118 41.620

34.316 41.728

35.173 42.598

34.368 40.951

29.799 43.253

29.553 43.241

29.309 44.171

28.433 45.221

28.539 46.525

27.577 47.563
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     ATOM 16604
                       GLY C 289
                   С
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                   N
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                   CB
                                                                                        С
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45
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                       GLU C 290
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                                                                                        O
                   OE1 GLU C 290
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                                                         67.245
                   OE2 GLU C 290
     ATOM 16618
                                                         66.185
                                                                  1.00 66.84
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                        THR C 292
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                                                                 1.00 83.48
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                    OG1 THR C 292
     MOTA
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5	ATOM	16645	CG2	THR C 292		23.660	44.683	69.301	1.00	82.75			С
3		16649		THR C 292		24.039	45.118	65.842		78.20			С
_	ATOM			THR C 292		24.152	46.206	65.281		76.52			0
	MOTA	16650		GLN C 293		23.212	44.153	65.414		77.10			N
	MOTA	16651				22.352	44.280	64.223		73.84			С
	MOTA	16653		GLN C 293		21.520		64.352		79.00			C
10	ATOM	16655		GLN C 293			45.562			85.11			Č
	MOTA	16658		GLN C 293		20.073	45.347	64.881					c
	MOTA	16661		GLN C 293		19.749	46.139	66.165		87.31		,	Ö
	MOTA	16662	OE1	GLN C 293		18.960	45.672	67.007		85.12			
	MOTA	16663	NE2	GLN C 293		20.347	47.329	66.308		86.21			N
15	ATOM	16666	С	GLN C 293		23.045	44.268	62.842		65.85			С
· .	ATOM	16667	0	GLN C 293		22.370	44.359	61.822		63.96			0
	MOTA	16668		GLN C 294	•	24.366	44.120	62.803		66.61			N
	MOTA	16670		GLN C 294		25.141	44.364	61.580		61.35			С
	ATÓM	16672	CB	GLN C 294		26.324	45.288	61.936	1.00	60.41			С
20		16675		GLN C 294		26.837	46.202	60.839		62.21			С
20	ATOM			GLN C 294		27.669	47.413	61.365		65.59			С
	ATOM	16678				28.765	47.713	60.847		59.99			0
	MOTA	16679		GLN C 294		27.138	48.107	62.373		65.49			N
	MOTA	16680		GLN C 294				60.985		56.94			C
	MOTA	16683	С	GLN C 294		25.627	43.036	61.710		58.82			ŏ
25	MOTA	16684	0	GLN C 294		25.912	42.085			46.60			N
•	MOTA	16685	N	SER C 295		25.718	42.958	59.668					Ċ
	MOTA	16687	CA	SER C 295		26.213	41.760	59.056		42.55			C,
	ATOM	16689	CB	SER C 295		25.079	40.909	58.628		40.84			
	ATOM	16692	OG	SER C 295		24.697	41.439	57.411		43.82			0
30	ATOM	16694	С	SER C 295		26.965	42.103	57.806		44.01			Ċ
	ATOM	16695	0	SER C 295		26.877	43.217	57.316		41.78			Ó
	ATOM	16696	N	PHE C 296		27.688	41.133	57.260		40.42			N
	ATOM	16698	CA	PHE C 296	* .	28.455	41.395	56.077		40.53			C
	ATOM	16700	CB	PHE C 296		29.870	41.876	56.413		42.71			. C
35	MOTA	16703	CG	PHE C 296		30.782	40.825	56.974	1.00	40.05			С
23	ATOM	16704		PHE C 296		31.588	40.081	56.147	1.00	43.51			С
	ATOM	16706		PHE C 296		32.406	39.148	56.647	1.00	36.06			C
•	ATOM	16708	CZ	PHE C 296		32.443	38.940	58.011	1.00	42.47			С
		16710		PHE C 296		31.674	39.657	58.822		37.71			С
40	MOTA	16712		PHE C 296		30.848	40.602	58.315		37.78			С
40	ATOM					28.455	40.127	55.332		42.08			С
	MOTA	16714	C	PHE C 296		28.030	39.122	55.906		46.21			0
	MOTA	16715	0	PHE C 296		28.908	40.167	54.070		40.78			N
	ATOM	16716	N	ARG C 297		28.958	38.974	53.211		44.56			C
4.5	ATOM	16718	CA	ARG C 297				52.123		44.33			Ċ
45	MOTA	16720	CB	ARG C 297		27.894	39.031			50.40			Č
	MOTA	16723	CG	ARG C 297		28.197	40.056	51.064		54.77			· C
	ATOM	16726	CD	ARG C 297		27.009	40.427	50.181		56.04	•		N
	ATOM	16729	NE	ARG C 297		27.370	41.445	49.195					_
	MOTA	16731	CZ	ARG C 297		26.505	42.187	48.535		50.69			C
50	ATOM	16732		ARG C 297		25.204	42.040	48.732		51.47			N
	ATOM	16735	NH2	ARG C 297		26.946	43.079	47.677		0 46.53			N
	MOTA	16738	С	ARG C 297		30.273	38.740	52.498		0 42.25	•		C
	ATOM		0	ARG C 297		31.035	39.648	52.215	1.0	0.47.66			0
	ATOM	16740	N	ILE C 298		30.518	37.488	52.194	1.0	0 41.06			N
55	ATOM	16742	CA	ILE C 298		31.679	37.115	51.439	1.0	0 41.71			С
	ATOM		CB	ILE C 298		32.517	36.104	52.264	1.0	0 38.04			С
•	MOTA	_		ILE C 298		31.858	34.741	52.331		0 39.06			С
	ATOM			ILE C 298		32.459		53.357		0 42.84			С
				2 ILE C 298		32.654	36.628	53.672		0 37.72			С
<i>(</i> 0	ATOM		C	ILE C 298		31.051	36.559	50.189		0 36.43			C
60	ATOM					29.989				0 39.29			0
	MOTA	16758	О	ILE C 298		27.707	33.993	50.200	0		•		-

-				mun			21 (25	36.727	49.041	1.00 41.37		N
5	ATOM	16759			C 299		31.675 31.098	36.225	47.769	1.00 42.98		C
	ATOM	16761			C 299			37.411	46.893	1.00 44.37		Ċ
	MOTA	16763			C 299		30.626	38.411	47.749	1.00 48.01		Ö
•	MOTA	16765			C 299		30.064		45.991	1.00 45.15		Ċ.
	MOTA	16767			C 299		29.455	37.062	47.050	1.00 38.51		c
10	ATOM				C 299		32.163	35.478	46.931	1.00 38.31		0.
	ATOM	16772			C 299		33.282	35.947		1.00 38.31		N
	ATOM	16773			C 300		31.834	34.309	46.557			C
	MOTA	16775			C 300		32.849	33.494	45.920	1.00 40.34		C
	ATOM	16777			C 300		33.019	32.177	46.685	1.00 40.87		c
15	MOTA	16779			C 300	٠.	32.051	31.162	46.204	1.00 34.13		Ċ
	MOTA	16782			C 300		32.254	29.851	46.922	1.00 36.30		C
	ATOM	16786			C 300		32.721	32.317	48.186	1.00 44.16		C
	ATOM	16790			C 300		32.440	33.216	44.505	1.00 40.76		
	MOTA	16791			C 300		31.254	33.277	44.220	1.00 39.41		0
20	ATOM	16792			C 301		33.426	32.905	43.645	1.00 44.04		N
	MOTA	16794			C 301		33.215	32.633	42.210	1.00 45.48		С
	MOTA	16796			C 301		34.199	33.429	41.340	1.00 47.46		C
	ATOM	16799			C 301		34.544	34.876	41.679	1.00 50.30	•	C.
	ATOM	16801			C 301		35.649	35.402	40.734	1.00 51.91		С
25	MOTA	16805			C 301		33.312	35.727	41.580	1.00 48.11	•	С
	ATOM	16809	С	LEU	C 301		33.338	31.183	41.734	1.00 46.00		С
	MOTA	16810	0	LEU	C 301	•	33.844	30.283	42.386	1.00 40.23		0
	MOTA	16811	N		C 302		32.905	30.973	40.516	1.00 47.02		N
	ATOM	16812	CA		C 302		32.898	29.626	39.965	1.00 45.68		C
30	ATOM	16814	CB		C 302		32.276	29.806	38.584	1.00 43.48		C
	ATOM	16817	CG		C 302		31.796	31.181	38.541	1.00 45.27		C
	ATOM	16820	CD		C 302		32.456	31.994	39.567	1.00 42.09		C
	ATOM	16823	С		C 302		34.331	29.104	39.891	1.00 48.54		С
	ATOM	16824	0		C 302		34:534	27.886	39.845	1.00 49.42		0
35	ATOM	16825	N		C 303		35.309	30.014	39.873	1.00 47.34		N
	ATOM	16827	CA		C 303		36.708	29.610		1.00 47.58		C
	ATOM	16829	CB		C 303		37.637	30.790	39.736	1.00 47.37		С
	MOTA	16832	CG		C ·303		37.910	31.131	38.293	1.00 45.62		С
	MOTA	16835	CD		C 303		36.936	32.113	37.717	1.00 45.06		C.
40	MOTA	16836			C 303		35.838	32.299	38.244	1.00 37.43		0
	MOTA	16837			C 303		37.334	32.747	36.617	1.00 50.52		N
	ATOM	16840	C		C 303		37.068	28.996	41.346	1.00 49.02		С
	ATOM	16841	0		C, 303		38.159	28.473	41.514	1.00 51.60		0
	ATOM	16842	N		C 304		36.169	29.052	42.316	1.00 49.47		N
45	ATOM	16844	CA		C 304		36.438	28.475	43.616	1.00 50.38		C
	MOTA	16846	CB		C 304		36.269	29.511	44.737	1.00 52.45		C
	MOTA	16849	CG		C 304		37.510	30.399	44.949	1.00 50.66		С
•	ATOM	16852			C 304		37.438			1.00 51.45		C
	MOTA	16853			C 304		38.235	31.881	43.210	1.00 51.29		0
50	ATOM	16854	NE2	GLN	C. 304	ļ	36.484	32.532	44.509	1.00 40.58		N
	ATOM	16857	С		C 304		35.606	27.249	43.939	1.00 51.95		С
	MOTA	16858	0		C 304			26.322	44.554	1.00 55.44		0
	MOTA	16859	N		C 305		34.328	27.212	43.574	1.00 56.29		N
_	MOTA	16861	CA		C 305		33.569	25.956	43.788	1.00 52.77		С
55	ATOM	16863	CB		C 305		32.064	26.151	44.100	1.00 50.80		C
	ATOM	16866	CG		C 305		31.206	26.929	43.131	1.00 44.82		C
	ATOM	16867			C 305		30.417	26.271	42.212	1.00 44.88		C
	ATOM	16869	CE1	TYR	C 30	õ	29.642	26.928	41.352	1.00 35.09		C
	ATOM	16871	CZ	TYR	C 30	5	29.594	28.271	41.368	1.00 36.83		С
60	ATOM	16872	ОН	TYR	C 30	5	28.748	28.910		1.00 41.33		0
	ATOM	16874	CE2	TYR	C 30	5	30.352	28.964	42.269	1.00 37.21		С

													*
5	ATOM	16876	CD2	TYR	C 305		31.149	28.290	43.155	1.00 38.78			С
	ATOM	16878	C.	TYR (€ 305		33.788	24.886	42.730	1.00 51.03			С
	ATOM	16879	0	TYR	C 305		33.369	23.774	42.952	1.00 53.32			0
	MOTA	16880	N	LEU (C 306		34.465	25.192	41.618	1.00 52.84			N
	ATOM	16882	CA	LEU (C 306		34.720	24.182	40.568	1.00 52.04			С
10	MOTA	16884	CB	LEU (C 306		34.395	24.713	39.181	1.00 54.77		•	С
	MOTA	16887	CG	LEU (C 306		32.909	24.805	38.761	1.00 51.54			Ç
	MOTA	16889	CD1	LEU (C 306		32.752	25.575	37.502	1.00 44.63			Ç
	ATOM	16893	CD2	LEU (C 306		32.350	23.442	38.555	1.00 52.67			Ċ
	MOTA	16897	С	LEU (C 306		36.187	23.850	40.620	1.00 56.99			С
15	MOTA	16898	0	LEU (C 306		37.008	24.666	40.199	1.00 57.98			0
	ATOM	16899	N	ARG (C 307		36.518	22.648	41.110	1.00 54.03			N
	MOTA	16901	CA	ARG (C 307		37.888	22.323	41.457	1.00 54.93			С
	ATOM	16903	CB	ARG (C 307		37.877	21.401	42.707	1.00 50.67			С
•	ATOM	16906	CG	ARG (C 307		39.207	20.794	43.096	1.00 51.43			С
20	MOTA	16909	CD	ARG (C 307		39.237	20.023	44.478	1.00 52.58			C
	MOTA	16912	NE	ARG (C 307		38.527	18.734	44.515	1.00 50.63			N
	MOTA	16914	CZ	ARG (C 307		38.946	17.609	43.939	1.00 47.81			С
	ATOM	16915	NH1	ARG	C 307		40.080	17.545	43.245	1.00 43.86			N
	ATOM	16918	NH2	ARG	C 307		38.217	16.525	44.053	1.00 50.54			N
25	ATOM	16921	С	ARG	C 307		38.629	21.735	40.241	1.00 58.15			С
	MOTA	16922	0		C 307		38.176	20.778	39.624	1.00 66.15			0
	ATOM	16923	N		C 308		39.755		39.870	1.00 59.79			N
	ATOM	16924	CA		C 308		40.546	21.788	38.744	1.00 59.10			С
	ATOM	16926	CB		C 308		41.640	22.856	38.523	1.00 56.70		•	C
30	ATOM	16929	CG		C 308		41.396.	23.964		1.00 56.84			C
	MOTA	16932	ĆD		C 308		40.358	23.515	40.488	1.00 59.81			С
	ATOM	16935	С		C 308		41.210	20.429	39.057	1.00 57.82			C
•	ATOM.	16936	0		C 308		41.842	20.326	40.111 38.160	1.00 54.21 1.00 58.91			O N
35	MOTA	16937 16939	N CA		C 309 C 309	•	41.077 41.652	19.441 18.095	38.319	1.00 58.31			C
33	ATOM	16941			C.309		40.551	17.114	38.722	1.00 65.79			c
•	ATOM	16943			C 309		39.588	17.770	39.716	1.00 66.84	·		Ċ
	ATOM	16947			C 309		39.779	16.616	37.484	1.00 67.52			c
	ATOM	16951	c		C 309		42.356	17.527	37.044	1.00 69.36			C
40	ATOM	16952	ŏ		C 309		42.656	18.262	36.125	1.00 69.68			0
	ATOM	16953	N		C 310		42.636	16.222	37.004	1.00 77.12			N
	ATOM	16955	CA		C 310		43.239	15.577	35.811	1.00 82.03			С
	ATOM	16957	CB	GLU	C 310		44.374	14.638	36.233	1.00 81.97			С
	MOTA	16960	CG	GLU	C 310		45.621	15.401	36.593	1.00 81.89			С
45	ATOM	16963	CD	GLU	C 310		45.544	16.821	36.063	1.00 80.73			С
	ATOM	16964			C 310		45.101	17.697	36.831	1.00 76.33			0
	MOTA	16965	OE2	GLU	C 310		45.908	17.048	34.889	1.00 75.15			0
	ATOM	16966	С		C 310		42.302	14.768		1.00 87.34			С
	MOTA	16967	0		C 310		41.793	13.708	35.306	1.00 84.75			0
50	ATOM	16968	N		C 311		42.089	15.239	33.670	1.00 93.03			N
	ATOM	16970	CA		C 311		41.249	14.483	32.746	1.00 97.25			С
.•	ATOM	16972	CB		C 311		41.259	15.044	31.311	1.00 99.29			С
	MOTA	16975	CG		C 311		40.444	14.163	30.329				С
	MOTA	16976			C 311		40.021	13.036	30.712	1.00101.63			0
55 ·	MOTA	16977			C 311		40.179	14.507	29.156	1.00 96.73			0
•	ATÓM	16978	C		C 311		41.744	13.036	32.777	1.00 98.09			C
	MOTA	16979	0		C 311		42.917	12.770	33.052	1.00 98.48			0
	ATOM	16980	N		C 312		40.840	12.109	32.493	1.00100.23			N
<i>6</i> Λ	ATOM	16982	CA		C 312		41.132	10.686		1.00101.33			C.
60	ATOM.	16984	CB		C 312		39.948	9.830	32.120 32.290	1.00101.66		_	C
	ATOM	16986	CGT	٧A٦	C 312	•	40.264	8.348	34.430	1.00105.68		-	C

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16990 CG2 VAL C 312
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                                                           42.428 10.292 31.906 1.00101.68
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CB THR C 314
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R C 315
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CD GLN C 316
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55
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                                                                                                                                    C
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        MOTA
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                             CD1 TYR C 320
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	MOTA	17094	CZ	TYR C 320		38.584	24.406	34.665		42.05			
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	MOTA	17097		TYR C 320		38.678	24.213	36.008		49.88			С
	ATOM	17099	CD2	TYR C 320		37.824	23.357	36.645		48.03			C
10	ATOM	17101	С	TYR C 320		35.796	19.427	37.713		50.65			С
	ATOM	17102	0	TYR C 320		35.243	18.517	37.104		50.64			0
	ATOM	17103	N	LYS C 321		35.681	19,611	39.042		48.99			N
	ATOM	17105	CA	LYS C 321		34.718	18.851	39.874		48.57			C
	ATOM	17107	CB	LYS C 321		35.394	17.846	40.803		51.22	•		С
15	MOTA	17110	CG	LYS C 321		35.994	16.592	40.130		59.14			C .
	MOTA	17113	CD	LYS C 321		36.034	15.363	41.092		60.36			; C
	ATOM	17116	CE	LYS C 321		36.528	14.083	40.379		61.02			С
	MOTA	17119	NZ	LYS C 321		36.887	12.972	41.327		60.51			· N
	ATOM	17123	С	LYS C 321		33.894	19.787	40.756		43.89			С
20	ATOM	17124	0	LYS C 321		34.388	20.685	41.391		48.32			0
	MOTA	17125	N	PHE C 322		32.614	19.570	40.806		45.71			N
	ATOM	17127	CA	PHE C 322		31.772	20.381	41.647		45.11			C
	MOTA	17129	CB	PHE C 322		30.325	19.886	41.516		39.38			С
	MOTA	17132	CG	PHE C 322		29.275	20.890	41.937		47.52			С
25	ATOM	17133	CD1	PHE C 322		29.280	22.186	41.454		52.42			С
	ATOM	17135	CE1	PHE C 322		28.318	23.066	41.839		46.38			С
	MOTA	17137	CZ	PHE C 322		27.334	22.671	42.708		41.85			. C .
	ATOM	17139	CE2	PHE C 322		27.315	21.436	43.176		38.98			С
	ATOM	17141	CD2	PHE C 322		28.266	20.535	42.801		38.92			С
30	ATOM	17143	С	PHE C 322		32.331	20.143	43.041		46.56	•		С
	ATOM	17144	oʻ	PHE C 322		32.334	18.998	43.496		55.34			0
	MOTA	17145	N	ALA C 323		32.827	21.180	43.713		40.68	-		N.
	ATOM	17147	CA	ALA C 323		33.267	21.030	45.100		36.91			C
	ATOM	17149	CB	ALA C 323		34.573	21.721	45.298		40.42			. C
35 .	ATOM	17153	С	ALA C 323		32.266	21.542	46.125		36.58			С
	ATOM	17154	0	ALA C 323		32.636	22.208	47.080		37.20			.0
	ATOM	17155	N	ILE C 324		30.989	21.267	45.943		37.33			N
	MOTA	17157	CA	ILE C 324		30.015	21.630	46.965		36.19			С
	MOTA	17159	CB	ILE C 324		29.023	22.599	46.424		39.76			C
40	MOTA	17161		ILE C 324		29.739	23.761	45.817		38.88	•		C
•	MOTA	17164		ILE C 324		28.812	24.873	45.598		45.35			C
	ATOM	17168		ILE C 324		28.083	23.152	47.527		42.74			C
	ATOM	17172	С	ILE C 324		29.353	20.321	47.267		41.52			
	MOTA	17173	0	ILE C 324		29.381	19.453	46.389		48.29			O N
45	ATOM	17174	N	SER C 325		28.788	20.145	48.473		43.90			C
	ATOM	17176	CA	SER C 325		28.161	18.864	48.868		44.02		*	C.
•	ATOM	17178	CB	SER C 325		29.154	17.696	48.881		45.54			0
	ATOM	17181	OG	SER C 325			18.073			56.81		*	-
	MOTA	17183	С	SER C 325		27.410	18.846	50.181		49.43		٠	C
50	ATOM	17184	0	SER C 325		27.528	19.750	51.015		54.04			. 0
	MOTA	17185	N	GLN C 326		26.624	17.786	50.339		55.37			N
	MOTA	17187	CA	GLN C 326	÷	25.797	17.593	51.509		59.34			C
	MOTA	17189	CB	GLN C 326		24.512	16.803	51.166		62.25			C
	ATOM	17192	CG	GLN C 326		24.703	15.342	50.735		66.34			C
55	MOTA	17195	CD	GLN C 326		23.421	14.731	50.154		73.31			C
	MOTA	17196		L GLN C 326		22.481	14.464	50.899		75.42			0
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*	ATOM	17201	0	GLN C 326		27.603	16.287	52.522		58.34			0
60	MOTA		N	SER C 327		26.017	17.211	53.862		60.79			N
	ATOM	17204	CA	SER C 327		26.599	16.804	55.118	1.00	58.82			С

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                      SER C 327
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	ATOM	17325	N	ILE C	337		36.198	27.799	49.915	1.00 53.2	6		N	
	ATOM	17327	CA	ILE C	337		35.714	29.050	50.421	1.00 54.8	8		С	;
	ATOM	17329	СВ	ILE C			34.812	28.821	51.617	1.00 59.9			С	
10	ATOM	17331		ILE C			33.605	28.021	51.167	1.00 62.6			С	
10	ATOM	17334		ILE C			33.536	27.873	49.654	1.00 65.7			Ċ	
								30.142	52.257	1.00 61.2			Č	
	MOTA	17338		ILE C			34.416			1.00 51.2			C	
	ATOM	17342	С	ILE C			36.884	29.853	50.861				0	
1.5	MOTA	17343	0	ILE C			36.885	31.076	50.754	1.00 60.3				
15	ATOM	17344	N	MET C			37.893	29.168	51.373	1.00 52.8			N	
	ATOM	17346	CA	MET C			39.058	29.859	51.874	1.00 45.9		٠,	C	
	MOTA	17348	CB	MET C			39.791	28.921	52.798	1.00 47.2			. 0	
	ATOM	17351	CG	MET C			39.048	28.822	54.095	1.00 46.3			C	
•	ATOM	17354	SD	MET C			39.827	27.707	55.154	1.00 50.0			S	
20	ATOM	17355	CE	MET C	338		41.323	28.450	55.484	1.00 38.5			С	
	ATOM	17359	С	MET C	338		39.946	30.388	50.744	1.00 42.5	2		C	:
	ATOM	17360	0	MET C	338		40.483	31.476	50.842	1.00 47.1	6		C)
	MOTA	17361	N	GLU C	339		40.093	29.619	49.685	1.00 36.7	8		N	j .
	ATOM	17363	CA	GLU C		٠.	40.815	30.034	48.514	1.00 37.1	7		C	;
25	ATOM	17365	CB	GLU C			40.806	28.877	47.493	1.00 43.9	2		C	;
	ATOM	17368	CG	GLU C			41.688	27.679	47.897	1.00 48.1			C	
	ATOM	17371	CD	GLU C			41.673	26.490	46.918	1.00 50.5			Ċ	
	ATOM	17372		GLU C		·	42.111	25.367	47.340	1.00 46.8				
	ATOM	17372		GLU C			41.232	26.671	45.751	1.00 41.2			· c	
30		17374	C.	GLU C			40.279	31.374	47.900	1.00 39.0			Ċ	
30	ATOM	17374		GLU C				31.896	46.962	1.00 42.3			Ċ	
	ATOM		0				40.832		48.402	1.00 42.0			. 1	
	ATOM	17376	N	GLY C			39.213	31.955					0	
	ATOM	17378	CA	GLY C			38.963	33.297	47.960	1.00 33.4			٠. ر	
25	MOTA	17381	С	GLY C			39.436	34.371	48.950	1.00 36.8				
35	ATOM	17382	,0	GLY C			39.491	35.574	48.678	1.00 33.1			C	
	ATOM	17383	N	PHE C			39.800	33.978	50.139	1.00 35.1			Į.	
	ATOM	17385	CA	PHE C			40.060	35.003	51.085	1.00 37.2			0	
	ATOM	17387	CB	PHE C			38.892	34.974	52.025	1.00 38.3			C	
40	MOTA	17390	CG	PHE C			37.579	35.096	51.327	1.00 40.3				
40	ATOM	17391		PHE C			36.751	33.993	51.165	1.00 41.8			(
	MOTA	17393			341		35.543	34.108	50.523	1.00 35.4			C	
	MOTA	17395	\mathbf{cz}	PHE C			35.160	35.341	50.042	1.00 35.2			(
	ATOM	17397		PHE C			35.976	36.453	50.198	1.00 27.3			C	
	ATOM	17399	CD2	PHE C			37.160	36.331	50.830	1.00 37.0			(
45	MOTA	17401	C	PHE C	341	•	41.393	34.881	51.842	1.00 37.7	2		C	
	ATOM	17402	0	PHE C	341		42.042	33.895	51.736	1.00 35.2	29		(
	ATOM	17403	N	TYR C	342		41.793	35.948	52.531	1.00 38.9	1		-1	1
	MOTA	17405	CA	TYR C	342		42.864	35.934	53.519	1.00 40.0	6		(7
	MOTA	17407	CB	TYR C			43.579	37.280	53.593	1.00 40.5	5 <u>2</u>		(2
50	MOTA	17410	CG	TYR C	342		44.730	37.363	54.555	1.00 39.3	32 ·		(3
	ATOM	17411	CD1	TYR C		٠.	45.634	36.362	54.621	1.00 37.4				2
	ATOM	17413		TYR C			46.694	36.415	55.487	1.00 39.8				2
	ATOM	17415	CZ	TYR C			46.880	37.469	56.308	1.00 40.	-			2
	ATOM	17416	ОН	TYR C			48.015	37.396	57.146	1.00 35.0				5
55	ATOM	17418		TYR C			45.972	38.527	56.273	1.00 33.0				2
33	ATOM	17420		TYR C			44.908	38.466	55.405	1.00 36.				3
	ATOM	17420	C	TYR C	-		41.948	35.832	54.690	1.00 30.				C,
		17422	0	TYR C			41.035	36.677	54.718	1.00 39.				Э. Э
•	MOTA													
60	MOTA	17424	N	VAL C			42.160	34.836	55.588	1.00 31.				N
60	MOTA	17426	CA	VAL C			41.279	34.548	56.731	1.00 32.1				C
	MOTA	17428	ĊВ	VAL C	343		40.744	33.094	56.729	1.00 34.	3		•	C

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C
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                         CG2 VAL C 343
      ATOM
              17434
                               VAL C 343
VAL C 343
VAL C 344
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                                                                           57.971
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                                                     42.126
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                         CG1 VAL C 344
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                                                                 37.469
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                               VAL C 344
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41.849
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40.403
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       ATOM 17466
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ATOM 17470
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42.133
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                         CD2 PHE C 345

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                         OD2 ASP C 346
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       ATOM 17486
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        ATOM
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34.093 32.572
33.300 32.324
36.758 35.693
35.541 35.923
37.520 35.768
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37.427
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SER C 357
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                                                      47.846
                                                              1.00 56.29
                      ALA C 358
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           17675
                  N
     ATOM
                      ALA C 358
                                                              1.00 56.23
                                     45.583
                                              38.848
                                                      46.722
                  CA
10 ATOM 17677
                      ALA C 358
                                      46.834
                                              39.538
                                                      47.217
                                                              1.00 56.89
                  CB
          17679
     MOTA
                                                                                    С
                      ALA C 358
ALA C 358
                                                              1.00 54.12
          17683 C
                                      45.994
                                              37.860
                                                      45.668
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                                                              1.00 56.22
                                                      44.708
                                      46.607 38.256
     MOTA
           17684
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                                                      45.852
                                                              1.00 54.48
                      CYS C 359
                                      45.696
                                              36.589
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           17685
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                                                              1.00 58.48
                      CYS C 359
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                      CYS C 359
                                      47.071
                                              34.636
                                                      45.479
     MOTA
           17689
                  CB
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                      CYS C 359
                                                      46.804
                                                              1.00 70.62
                                      46.287
                                              33.673
     ATOM
           17692
                  SG
                      CYS C 359
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                                                      44.441
                                                              1:00 55.69
                                                                                    C
                  С
           17693
     MOTA
                      CYS C 359
                                     45.065 33.670
                                                      43.872
                                                              1.00 58.26
                                                                                    0
           17694
                  0
     MOTA
                                                              1.00 52.56
                                                                                    N
                                      43.646
                                                      44.698
20
     ATOM
           17695
                  N
                      HIS C 360
                                             35.200
                                                              1.00 47.84
                                                                                    C
                                              34.444
                                                      44.313
                 · CA · HIS C 360
           17697
                                   42.458
     MOTA
                                  41.228
40.456
40.527
39.725
                                                      45.062
                                                              1.00 44.33
                                                                                    С
                      HIS C 360
                                              34.911
          17699
     MOTA
                  CB
                                                                                    С
                                              35.978
                                                      44.368
                                                              1.00 36.46
                  CG HIS C 360
     ATOM 17702
                                                      44.749
                                                              1.00 35.80
                                                                                    N
                                              37.304
                  ND1 HIS C 360
     ATOM 17703
                                                      43.980
                                                               1.00 32.97
                                                                                    C
                  CE1 HIS C 360
                                              38.021
25
     ATOM 17705
                                   . 39.146
                  NE2 HIS C 360
                                              37.205
                                                      43.108
                                                               1.00 35.99
                                                                                    N
     ATOM 17707
                                                               1.00 24.33
                                                      43.334
                                                                                    C
     ATOM 17709
                  CD2 HIS C 360
                                      39.583
                                              35.920
                                                      42.837
                                                               1.00 48.33
                                                                                    C
                       HIS C 360
                                      42.149
                                              34.453
     ATOM 17711
                  С
                                                              1.00 55.09
                                              35.472 42.212
                                                                                    0
                                      41.972
           17712
                       HIS C 360
     ATOM
                  0
                                                      42.301
                                                               1.00 48.18
30
                                      42.049
                                              33.269
     ATOM
           17713
                  N
                       VAL C 361
                                                               1.00 49.01
                      VAL C 361
                                      41.775
                                              33.081
                                                      40.913
     MOTA
           17715
                   CA
                                  41.75
41.585
41.177
42.857
40.511
39.424
40.623
39.418
                                                      40.711
                                                               1.00 46.22
                      VAL C 361
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           17717
     MOTA
                   CB
                   CG1 VAL C 361
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                                                      39.315
                                                               1.00 51.10
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                                                               1.00 47.29
     ATOM
           17723
                   CG2 VAL C 361
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                                                     40.444
                                                               1.00 51.23
                                                                                    С
                                              33.766
35
          17727
                      ·VAL C 361
     MOTA
                   С
                                              33.400 40.904
                                                              1.00 56.14
                       VAL C 361
     MOTA
          17728
                                                      39.552
                                                               1.00 52.97
                       HIS C 362
                                              34.748
     ATOM 17729
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                                      39.418
                                              35.335
                                                      38.940
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                      HIS C 362
     ATOM 17731
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                       HIS C 362
                                      38.911
                                              36.603
                                                      39.652
                                                               1.00 62.76
     ATOM 17733
                   CB
                                                      39.721
                                                               1.00 66.49
40
     ATOM 17736
                   CG
                       HIS C 362
                                      39.899
                                              37.726
                                                      40.807
                                      40.724
                                              37.924
                                                               1.00 69.80
                   ND1 HIS C 362
     ATOM
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                   CE1 HIS C 362
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                                              38.984 40.598
                                                               1.00 70.34
     MOTA
           17739
                                                               1.00 71.05
                   NE2 HIS C 362
                                      41.181 39.486
                                                      39.417
           17741
     MOTA
                   CD2 HIS C 362
                                              38.721
                                                      38.849
                                                               1.00 71.53
           17743
                                      40.187
     MOTA
                                                                                    C
45
                       HIS'C 362
                                      39.569 35.585
                                                     37.467
                                                               1.00 56.16
           17745
                   C
     MOTA
                                              35.203 36.886
                                                                                    0
                       HIS C 362
                                      40.553
                                                               1.00 55.35
     MOTA
           17746
                   0
                                                               1.00 62.61
                                      38.559 36.210 36.869
                                                                                    N
     MOTA
           17747
                   N
                       ASP C 363
     ATOM 17749 CA ASP C 363
                                              36.570
                                                      35.436
                                                               1.00 63.83
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                                   . 37.395
                      ASP C 363
                                              35.908
                                                      34.686
                                                               1.00 62.33
     ATOM 17751
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                                      36.028
                                              36.093
                                                       35.405
                                                               1.00 67.13
                                                                                    С
 50
     ATOM 17754
                   CG ASP C 363
                   OD1 ASP C 363
                                      35.956
                                              36.855
                                                       36.408
                                                               1.00 60.86
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     ATOM 17755
                                                               1.00 63.80
                   OD2 ASP C 363
                                      34.969
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                      ASP C 363
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                                                       35.425
                                                               1.00 62.69
      MOTA
           17757
                   С
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                                                               1.00 65.13
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                                      38.327
     MOTA
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 55
                       GLU C 364
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     MOTA
                   N
                       GLU C 364
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                                              40.178
                                                       34.212
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           17761
      MOTA
                   CA
                                      38.753
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                                                       32.793
                                                               1.00 60.33
           17763
                       GLU C 364
                   CB
      ATOM
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                   CG
                       GLU C 364
      MOTA
                                              42.269
                                                               1.00 70.09
                       GLU C 364
                                                       30.943
           17769
                   CD
                                      38.714
      MOTA
                                                       30.055
                                              41.370
                                      38.632
                                                               1.00 68.45
. 60
            17770
                   OE1 GLU C 364
      MOTA
                                  . 39.216
                                              43.417
                                                       30.749
                                                               1.00 72.62
            17771
                   OE2 GLU C 364
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5	ATOM	17772	С	GLU C 364	1	37.097	40.860	34.703	1.00	55.57			(3
,		17773		GLU C 364		37.111	41.994	35.171	1.00	55.50)
	ATOM	17774		PHE C 365		35.971	40.175	34.628	1.00	50.41			1	N
	MOTA	17776		PHE C 36!		34.702	40.825	34.944	1.00	48.24			. (3
	MOTA			PHE C 365		33.671	40.470	33.882	1.00	48.33			(3
10	MOTA	17778		PHE C 36		34.219	40.334	32.501	1.00	48.95			(C -
10	ATOM	17781		PHE C 36		34.692	39.123	32.072	1.00	49.95			(С
	ATOM	17782				35.199	38.950	30.789	1.00	53.08			(С
	ATOM	17784		PHE C 365		35.233	39.991	29.912		55.82			(C,
	ATOM	17786		PHE C 36		34.750	41.271	30.319		56.84				c [']
	MOTA	17788				34.730	41.424	31.616		56.84				С
15	MOTA	17790		PHE C 36		34.243		36.292		45.78				C.
	ATOM	17792	C	PHE C 36			40.457	36.576		49.51				0
	ATOM	17793	0	PHE C 36		32.976	39.663	37.105		45.57		•		N
_	ATOM	17794	N	ARG C 36		34.682	39.240	38.385		41.73				С
	ATOM	17796	CA	ARG C 36		34.121	38.013	38.194		38.80				С
· 20	ATOM	17798	CB	ARG C 36		33.243		38.384		37.22				C
	MOTA	17801	CG	ARG C 36		31.822	38.352	38.128		40.56				
	ATOM	17804	CD	ARG C 36		30.802	37.311	37.537		48.25				N
	ATOM	17807	NE	ARG C 36		31.257	36.052			47.05				С
	MOTA	17809	CZ	ARG C 36		30.432	35.033	37.321		44.28				N
25	MOTA	17810		ARG C 36		29.168	35.161	37.641		53.80				N.
	MOTA	17813		ARG C 36		30.852	33.894	36.787		42.95				c
	ATOM	17816	С	ARG C 36		35.212	38.904	39.367		47.17				ŏ
	MOTA	17817	0	ARG C 36		36.107	38.169	39.041		45.66				N
	MOTA	17818	Ŋ	THR C 36		35.105	39.427	40.577		47.80				c
30	ATOM	17820	CA	THR C 36		36.140	39.279	41.588		51.39				c
	MOTA	17822	CB	THR C 36		36.868	40.622	41.749		57.38	•			õ
	MOTA	17824	OG1	THR C 36		38.131	40.423	42.363		56.23				c
	MOTA	17826		THR C 36			41.538	42.774		46.46				c
	ATOM	17830	С	THR C 36		35.492	38.965	42.905		54.55				ō
35	MOTA	17831	0	THR C 36		34.522	39.642	43.277		39.88				N
	MOTA	17832	N	ALA C 36		35.993		43.640		32.52				C
•	MOTA	17834	CA	ALA C 36		35.375	37.681	44.909 45.526		37.31				Č
	MOTA	17836	CB	ALA C 36		36.048	36.619			39.83				c
	MOTA	17840	С	ALA C 36		35.389	38.935	45.813		44.69				ō
40	MOTA	17841	0	ALA C 36		36.237	39.822	45.723 46.715		43.60				N
	MOTA	17842	N	ALA C 36		34.440	39.005			40.45				c
	MOTA	17844	CA	ALA C 3		34.275	40.200	47.502 46.899		43.87				c
	MOTA	17846	CB	ALA C 3		33.188	40.996	48.946		37.91				Ċ
٠. ـ	ATOM	17850	С	ALA C 3		33.937	39.926	49.352		37.55				ō
45	ATOM	17851	0	ALA C 3		33.672	38.782			36.68				N
	MOTA	17852	N	VAL C 3		33.960				36.40				C
	MOTA	17854	CA	VAL C 3		33.625	41.058	51.097		34.82				Ċ
	ATOM	17856	CB	AMP C 3.			40.835	51.938		39.75				c
	MOTA	17858		VAL C 3		34.375		53.345	1.00	40.98				č
50	MOTA	17862		VAL C 3		35.455		51.558		38.45				c
	ATOM	17866	С	VAL C 3		33.125		51.368						ō
	MOTA	17867		VAL C 3		33.886				26.92				Ņ
	MOTA		N	GLU C 3		31.840		51.674		44.21				C
	MOTA			GLU C 3		31.246				47.61				Ċ
55	MOTA	17872		GLU C 3		30.441		50.559		51.18				č
	MOTA			GLU C 3		31.339				54.46	-			c
	MOTA			GLU C 3		30.714				57.83				0
	ATOM			GLU C 3		31.465				64.47				0
•_	ATOM			Grac 3		29.479				63.16				C
60	MOTA	17881	С	GLU C 3		30.337				48.24				0
•	MOTA	17882	0	GLU C 3	71	29.893	43.081	53.576	1.00	47.20				U

_			_			20. 262	45 211	52 440	3 00 50 00		N
5	MOTA	17883	N	GLY C 372	-	30.062	45.311	53.440	1.00 50.29		C
	MOTA	17885	CA	GLY C 372		29:156	45.560	54.560	1.00 50.67		c
	MOTA	17888	С	GLY C 372		29.149	47.025	54.947	1.00 50.50		
	MOTA	17889	0	GLY C 372		29.884	47.806	54.361	1.00 51.93		0
•	ATOM	17890	N	PRO C 373		28.353	47.431	55.934	1.00 52.13		N
10	MOTA	17891	CA	PRO C 373		27.466	46.568	56.733	1.00 47.64		С
	ATOM	17893	CB ·	PRO C 373		27.318	47.351		1.00 51.45		С
	MOTA	17896	CG	PRO C 373		27.992	48.699	57.790	1.00 49.65		C
	ATOM	17899	CD	PRO C 373		28.278	48.839	.56.356	1.00 47.50		C
	ATOM	17902	С	PRO C 373		26.077	46.434	56.223	1.00 46.53		C
15	ATOM	17903	0	PRO C 373		25.632	47.293	55.527	1.00 45.34		0
	MOTA	17904	N	PHE C 374		25.398	45.365	56.607	1.00 52.57	•	N
	MOTA	17906	CA	PHE C 374		24.028	45.097	56.195	1.00 50.90		C
•	ATOM	17908	CB	PHE C 374		23.894	43.751	55.484	1.00 49.66		, C
	ATOM	17911	CG	PHE C 374		24.437	43.797	54.115	1.00 48.09		С
20	ATOM	17912	CD1	PHE C 374		25.718	43.429	53.899	1.00 39.08		С.
	ATOM	17914		PHE C 374		26.255	43.495	52.658	1.00 42.90		С
	ATOM	17916	CZ	PHE C 374		25.507	43.947	51.602	1.00 42.40		C
	ATOM	17918		PHE C. 374		24.192	44.339	51.799	1.00 39.12	•.	С
	ATOM	17920		PHE C 374		23.660	44.272	53.042	1.00 42.78		C
25	ATOM	17922	C	PHE C 374		23.203	45.056	57.387	1.00 52.02		С
22	ATOM	17923	ō	PHE C 374		23.499	44.353	58.298	1.00 54.34		0
	ATOM	17924	N	VAL C 375		22.141	45.825	57.369	1.00 64.41		N
	MOTA	17926	CA	VAL C 375		21.259	45.867	58.496	1.00 65.17		С
	ATOM	17928	СВ	VAL C 375		20.319	47.035	58.465	1.00 65.29		·C
30	ATOM	17930		VAL C 375		18.943	46.570	58.832	1.00 62.93		С
50	ATOM	17934		VAL C 375		20.850	48.116	59.416	1.00 68.23		С
	ATOM	17938	C	VAL C 375		20.504	44.604	58.423	1.00 65.98		С
	ATOM	17939	Ö	VAL C 375		19.770	44.346	57.465	1.00 61.21		o ·
	ATOM	17940	N .			20.735	43.830		1.00 69.92		N
35	ATOM	17942	CA	THR C 376		20.191	42.515	59.661	1.00 72.22		С
55	ATOM	17944	CB	THR C 376		21.334	41.602	59.808	1.00 68.57		С
-	ATOM	17946		THR C 376		22.053	41.618	58.582	1.00 71.14		0
	ATOM	17948		THR C 376		20.874	40.181	59.945	1.00 74.54	•	С
	ATOM	17952	C	THR C 376		19.394	42.475	60.931	1.00 76.89		C
40	ATOM	17953	ŏ	THR C 376		19.568	43.345	61.802	1.00 77.58		0
40	ATOM	17954	N	LEU C 377		18.515	41.483	61.041	1.00 78.66		N
	ATOM	17956	CA	LEU C 377		17.779	41.340	62.271	1.00 81.96		С
	ATOM	17958	CB	LEU C 377		16.384	42.007	62.166	1.00 82.78		c ·
	ATOM	17961	CG	LEU C 377		16.197	43.562	62.077	1.00 80.18		С
45	MOTA	17963		LEU C 377		14.947	43.957	62.853	1.00 78.29		C
43	MOTA	17967		LEU C 377		17.354	44.441	62.577	1.00 78.91		Ċ
٠.	ATOM	17971	CDZ	LEU C 377		17.724	39.892	62.815	1.00 85.19		Ċ
	MOTA	17972	o	LEU C 377					1.00 84.41		O.
				ASP C 378		17.759	39.855	64.146	1.00 85.34		N
50	ATOM	17973	N	ASP C 376		17.597	38.638	64.925	1.00 86.48		ċ
50	ATOM	17975		ASP C 378		16.107	38.328	65.098	1.00 87.44		Č
	ATOM	17977	CB			15.461	39.248	66.154	1.00 89.47		Č
	MOTA	17980	CG	ASP C 378	•	14.462		65.855			Ö
	MOTA	17981		ASP C 378		15.931	39.308	67.324	1.00 84.37		Ö
c c	ATOM	17982		ASP C 378			37.522		1.00 85.14	•	C·
55	MOTA	17983	C	.ASP C 378		18.427	36.486	63.887	1.00 81.67		0
	ATOM	17984	0	ASP C 378		17.942 19.722	37.805	64.374	1.00 81.67		N
	ATOM	17985	N	MET C 379			•				C
	ATOM	17987	CA	MET C 379		20.750	36.965	63.819	1.00 82.56 1.00 81.97		c
C 0	ATOM	17989	CB	MET C 379		22.027	37.805	63.684	1.00 81.97		c
60	ATOM	17992	CG	MET C 379		21.955	38.836	62.581			· s
	ATOM	17995	SD	MET C 379		23.553	39.475	62.065	1.00 83.45		٥

					270	23.573	41.080	62.930	1.00	84.33		С
5	ATOM	17996.		MET C		21.010	35.728	64.668		84.75		С
	MOTA		С	MET C			34.618	64.133		82.43		0 .
	ATOM .		0	MET C		21.060		65.986		87.40		Ν.
	ATOM	18002	N	GLU C		21.163	35.920			87.60		
	MOTA	18004	CA	GLU C		21.555	34.840	66.914		89.46		C C
10	ATOM	18006	CB	GLU C		21.977	35.423	68.276				c
	ATOM	18009	CG	GLU C	380	22.952	34.592	69.137		93.46		Ċ
	ATOM		CD	GLU C	380	23.920	33.680	68.372		95.12		
	ATOM			GLU C		25.124	34.033	68.271		90.03		0
	ATOM			GLU C		23.480	32.596	67.888		96.29		0 .
15	MOTA		C	GLU C		20.459	33.763	67.031		86.12		С
15			o	GLU C			32.687	67.584		86.59		0
	MOTA	18017		ASP C		19.274	34.075	66.511	1.00	83.49		N
	MOTA			ASP C			33.064	66.258	1.00	81.88		С
	ATOM	18019	CA	ASP C		16.884	33.717	66.074	1.00	84.33		С
	ATOM	18021	CB	ASP C		16.354	34.306		1.00	88.13		С
20	ATOM .	18024	CG			17.009	34.123	68.400		92.81		0
	MOTA	18025	ODT	ASP C	, 301	15.285	34.957	67.412		96.45		0
	MOTA	18026		ASP C			32.177	65.026		77.79		С
	MOTA	18027	С	ASP (18.542	31.347	64.663		73.78		0
•	MOTA	18028	0		381	17.711	32.376	64.374		76.40		N
25	MOTA	18029	N		382	19.691		63.331		74.85		C .
	MOTA	18031	CA		382	20.187				75.98		C
	ATOM	18033	CB		382.	20.891		62.222		81.03		s
	ATOM	18036	SG		382	19.819		61.620	1.00	71.07		Ċ
	ATOM	18037	С		382	21.192		63.948	1.00	71.77		ó
30	MOTA	18038	0		C 382	21.755		63.284	1.00	70.20		N
	MOTA	18039	N	GLY (C 383	21.432		65.230		70.20		C
	MOTA	18041	CA		C 383	22.315		65.987		67.41		Ċ
٠.	ATOM	18044	С		C 383	21.508		66.386		63.32		o
	MOTA	18045	0		C 383	20.307		66.344		70.66		N
35	MOTA .	18046	N		C 384	22.173		66.777		70.77		C
	ATOM	18048	CA		C 384	21.524		67.055		73.27		Č
	MOTA	18050	CB		C 384	22.069		66.056		78.48		Č
	MOTA	18053	CG		C 384	21.523		66.237		81.09		Č
	ATOM	18054		LTYR		20.204		65.946		85.92		č
40	MOTA	18056	CE.	L TYR	C 384	19.67	22.472	66.103				Č
,	ATOM	18058	CZ	TYR	C 384	20.465				86.01		ŏ
	ATOM	18059	OH	TYR	C 384	19.876		66.701		0 90.24		c
	ATOM		CE	2 TYR	C 384	21.805				0 85.31		C
•	ATOM		CD:	2 TYR	C 384	22.322				0 81.62		C
45	ATOM		С	TYR	C 384	21.81	5 25.839			0 69.90		0
	ATOM		0	TYR	C 384	22.87				0 72.05		
	ATOM		N		C 385	20.91				0 70.22	٠	N C
	ATOM		CA	ASN	C 385	21.07	5 24.714			0 71.13		
•	ATOM		СВ		C 385	20.18	9 25.677	71.312		0 69.28		C
50	ATOM		CG	ASN	C 385	20.76	0 27.093			0 71.39		C
JU .	ATOM			1 ASN	C 385	21.95		71.578		0.73.33		. 0
	ATOM				C 385	19.92		71.047	1.0	0 59.22		N
			C		C 385	20:88		71.086		0 73.98	-	C
	ATOM		Ö		C 385	19.84	4 22.617		1.0	0 78.23		0
5.5	ATOM				C 385	21.76			1.0	0 70.20		0
55	ATOM			GLU		24.81			1.0	0 49.83		N
	ATOM		N			24.83				0 49.27		С
	ATOM		CA			24.71				0 52.47		С
	MOTA					24.17				0 53.06		С
60	ATON	_				23.83				0 54.58	•	Ċ
60	1OTA					23.12				00 58.12		0
	MOTA	4 18093	OE.	:1 GLU	ז ע	. 23.12			,			

		-									•			
5	MOTA	18094	OE2	GLU	D	1		24.276	12.444	10.373	1.00 51.77			0
Ĭ.	ATOM	18095	С	GLÜ		1		26.172	9.309	14.292	1.00 53.40			С
	ATOM	18096	0	GLU		1		27.170	9.803	14.821	1.00 62.53			0
	ATOM	18099		VAL		2		26.219	8.207	13.540	1.00 50.49			N
		18101	CA	VAL		2		27.451	7.883	12.839	1.00 47.46			С
10	ATOM	18103	CB	VAL		2		27.878	6.495	13.081	1.00 48.05	•		C
10	ATOM	18105		VAL		2		28.636	6.435	14.387	1.00 43.66			C
	ATOM	18109		VAL		2		26.682	5.606	13.046	1.00 48.85			С
	ATOM	18113	C	VAL		2		27.416	8.076	11.318	1.00 46.38			С
•	ATOM	18114	0	VAL		2		26.397	8.224	10.710	1.00 45.59			0
.15	ATOM	18115	N	ASN		3		28.589	8.071	10.719	1.00 46.83			· N
.13	ATOM	18117	CA	ASN		3		28.728	8.117	9.292	1.00 48.82			C,
-	ATOM	18119	СВ	ASN		3		28.844	9.528	8.743	1.00 47.44			С
	ATOM	18122	CG	ASN		3		27.547	10.251	8.771	1.00 50.24			С
	ATOM	18123		ASN		3		27.033	10.674	7.743	1.00 45.24			0
20 ⁻	ATOM	18124		ASN		3		26.998	10.409	9.963	1.00 53.88			N
20	ATOM	18127	С	ASN		3		30.011	7.,423	9.016	1.00 45.35		•	С
	ATOM	18128		ASN		3		30.876	8.042	8.462	1.00 .56.01			0
	ATOM	18129	ō	LOL		4		30.649	3.658	7.253	1.00 41.49			0
.•	ATOM	18130	C	LOL		4		31.616	4.701	7.302	1.00 44.31	•		, C
25	MOTA	18131	CA	FOF		4		31.464	5.422	8.643	1.00 44.47			С
23	MOTA	18132	N.	LOL		4		30.059	5.809	8.714	1.00 40.56			N
	ATOM	18133	СВ	FOF		4		31.620	4.400	9.742	1.00 39.73			C
	ATOM	18134	CG	POF		4		31.782		11.041	1.00 42.24			С
	ATOM	18135		LOL		4		32.929	6.168	11.002	1.00 38.09			С
30.	MOTA	18136		LOL		4		32.012	4.153	12.156	1.00 44.46			С
50	ATOM	18137	0	ALQ		5		33.539	6.138	4.922	1.00 46.58			0
	ATOM	18138		ALQ		5		32.895	5.448	4.118	1.00 40.59			С
	ATOM	18139	CA	ALQ		5		31.531	4.899	4.429	1.00 34.48			С
	ATOM	18140	CM	ALQ		5		31.262	5.085	5.904	1.00 25.68			С
35	ATOM	18141	СВ	ALQ		.5		30.525	5.761	3.689	1.00 32.81			, C
70	ATOM	18142	N	ALA		6	•	33.833	4.377	4.106	1.00 47.34	•		N
	ATOM	18144	CA	ALA		6		35.183	4.871	3.785	1.00 46.63			С
	ATOM	18146	CB	ALA	D	6		35.992	3.752	3.209	1.00 48.42			С
	ATOM	18150	С	ALA	· D	6		35.139	6.050	2.825	1.00 48.53			С
40	MOTA	18151	0	ALA	D	6		34.387	6.073	1.850	1.00 41.51			0
	ATOM	18154	N	GLU	D	7		35.936	7.053	3.153	1.00 57.71			N
	ATOM	18156	CA	GLU.	D	7		36.170	8.193	2.282	1.00 61.39			С
	ATOM	18158	CB	GLU	D	7		37.103	9.150	2.997	1.00 63.36			С
	ATOM	18161	CG	GLU	D	7		36.554	10.567	3.088	1.00 69.77			C
45	.ATOM	18164	CD	GLU	D	7		37.556	11.591	3.638	1.00 72.88			C
	MOTA	18165	OE1	GLU	D	7		37.130	12.437	4.470	1.00 71.19			0
	ATOM	18166	OE2	GLU	D	7		38.753	11.548	3.245	1.00 71.30			Ó
	ATOM	18167	С	GLU	D	7		36.746	7.878	0.873				С
	ATOM.	18168	0	GLU	D	7		36.460	8,610	-0.067	1.00 59.17			O
50	ATOM	18169	N	PHE	D	8		37.554	6.833	0.708	1.00 64.51			N
	ATOM	18171	CA	PHE	D	8		38.046	6.472	-0.636	1.00 66.42			С
	MOTA	18173	CB	PHE	D	8		37.450	5.145	-1.093	1.00 61.61	•		C
	ATOM	18176	CG	PHE	D	8		38.061	4.586	-2.379	1.00 58.86			С
	ATOM	18177	CD1	PHE	D	8		37.441	4.769	-3.602	1.00 59.33			C
55	ATOM	18179	CE1	PHE	D	8		37.986	4.253	-4.767	1.00 58.96			C
	MOTA	18181	CZ	PHE	D	8		39.174	3.536	-4.731	1.00 60.39	•		С
	MOTA	18183		PHE		8		39.800	3.345	3.536	1.00 58.60			С
	MOTA	18185	CD2	PHE	D	8		39.239	3.869	-2.355	1.00 59.06			С
	ATOM	18187	С	PHE		8		37.706	7.526	-1.692	1.00 70.25			С
60	ATOM	18188	0	PHE		8		36.951	7.302	-2.641	1.00 73.78			0
	MOTA	18189	OXT	PHE	D	8		38.159	8.667	-1.670	1.00 76.04			0

								•						
5	ATOM	18190	N.	GLU I	E	1		3.521	56.829	27.990	1.00 51.90		N	
	MOTA	18192	CA	GLU I	E	1		4.813	56.347	27.405	1.00 53.95		C.	
	MOTA	18194	CB	GLU :	E	1		4.748	54.908	26.863	1.00 52.89		С	
	MOTA	18197	CG ·	GLU :	E	1		6.020	54.441	26.144	1.00 54.53		С	
	MOTA	18200	CD	GLU :	E	1		5.940	53.023	25.544	1.00 61.12		С	
10	ATOM	18201	OE1	GLU :	E	1		4.802	52.481	25.400	1.00 68.56	•	0	
10	ATOM	18202	OE2	GLU :	E	1		7.009	52.427	25.193	1.00 55.04		Ο.	
	ATOM	18203	С	GLU		1		5.206	57.280	26.290	1.00 56.24		С	
	ATOM	18204	ō	GLU		1		4.726	57.179	25.177	1.00 58.77		0	
	ATOM	18207	N	VAL		2		6.069	58.225	26.625	1.00 60.38		. И	
15		18209	CA	VAL		2		6.748	59.058	25.641	1.00 55.03		C.	
.15	ATOM	18211	CB	VAL		2		7.513	60.074	26.359	1.00 53.73		С	
	ATOM			VAL		2	•	6.581	60.848	27.263	1.00 55.96		C	
•	MOTA	18213				2		8.615	59.394	27.171	1.00 56.70		c	
	ATOM	18217		VAL					58.285	24.804	1.00 54.06		C	
-00	MOTA	18221	С	VAL		2		7.758		25.214	1.00 51.79		Ö	
20	ATOM.	18222	0.	VAL		2		8.268	57.267	•	1.00 51.75		N	
	MOTA	18223	N	ASN		3	•	8.053	58.785	23.618	1.00 49.08		C	
	ATOM	18225	CA	ASN		3		9.062	58.167	22.787		. •	c	
	MOTA	18227	CB	ASN		3		8.502	56.972	22.011	1.00 52.23		C	
· ·	MOTA	18230	CG	ASN		3		8.790	55.632	22.678	1.00 58.18	•		
25	MOTA	18231		ASN		3		9.955	55.264	22.882	1.00 65.86		0	
	MOTA	18232	ND2	ASN	E	3		7.724	54.885	23.009	1.00 59.14		N	
	MOTA	18235	Ċ	ASN	E	3		9.599	59.235	21.836	1.00 48.29		C	
	ATOM	18236	0	ASN	E	3		9.547	59.112	20.605	1.00 43.64		0	
	MOTA	18237	O	\mathbf{ror}	E	4		12.598	62.494	21.688	1.00 44.76	• .	0	
30	ATOM	18238	С	LOL	E	4		$\cdot 11.793$	61.498	21.082	1.00 36.75		С	
	ATOM	18239	CA	LOL	E	4		10.394	61.683	21.640	1.00 39.29		C	
	ATOM	18240	N	LOL	E	4		10.081	60.567	22.545	1.00 35.78	•	N	
	ATOM	18241	CB	\mathbf{ror}	E	4		10.243	62.899	22.530	1.00 30.76		C	
•	ATOM	18242	CG	LOL	E	4		8.730	62.693	22.652	1.00 40.35		С	
·35	ATOM	18243	CD2	LOL	E	4		8.185	62.234	21.296	1.00 31.81		C.	
	ATOM	18244	CD1	LOL	E	4		8.003	63.914	23.151	1.00 38.31		С	
	MOTA	18245	0	ALQ	E	5		12.574	60.630	18.017	1.00 56.62		0	
	ATOM	18246	С	ALQ	E	5		12.792	61.258	19:046	1.00 45.00		С	
	MOTA	18247	CA	ALQ	E	5		13.506	60.509	20.107	1.00 39.17		С	
40	MOTA	18248	CM	ALQ	E	5		12.383	59.943	20.954	1.00 33.18		С	
•	MOTA	18249	CB	ALQ	E	5		14.198	59.370	19.382	1.00 38.30		С	
	ATOM	18250	N	ALA	E	6		13.763	61.587	17.911	1.00 53.06		N	
	ATOM	18252	CA	ALA	E	6		13.416	62.316	16.681	1.00 48.77		С	
	MOTA	18254	СВ	ALA	E	6		14.238	63.578	16.590	1.00 46.81		С	
45	ATOM	18258	С	ALA	E	6		13.739	61.376	15.550	1.00 56.62		. C	
•	MOTA	18259	0	ALA	E	6	. •	14.884	61.001	15.355	1.00 60.60		О	
	ATOM	18262	N.	GLU	E	7		12.718	60.941	14.836	1.00 66.83	•	N	
	ATOM	18264	CA	GLU	E	7		12.894	60.209	13.578	1.00 70.79		С	
	ATOM	18266	CB	GLÚ		7		11.658	60.366	12.670	1.00 71.58		, C	;
50	ATOM	18269	CG	GLU		. 7		11.195	58.999	12.147	1.00 74.78	,	С	;
50	ATOM	18272	CD	GLU		7		9.767	58.949	11.583	1.00 77.65	• •	C	:
	ATOM	18273		GLU		7		9.502	59.494	10.475	1.00 71.21		0)
	ATOM	18274		GLU		7		8.907	58.325	12.252	1.00 77.08		0)
	ATOM	18275	C	GLU		7		14.184	60.468	12.764	1.00 72.67		С	:
55		18276	ő	GLU		7		15.094	59.622	12.765	1.00 77.73		0	
))	ATOM	18277	N	PHE		8		14.297	61.598	12.076	1.00 75.16		N	
	ATOM		CA	PHE		8		15.396	61.740	11.113	1.00 80.96		C	
	MOTA	18281	CB :			8		16.737	61.952	11.801	1.00 82.87		· c	
	ATOM	18284	CG	PHE		8		17.803	62.573		1.00 81.73		Ċ	
60	MOTA	18285		PHE		8		18.769	61.793		1.00 83.54		Č	
UU.	ATOM	18287		PHE		8		19.751	62.381		1.00 81.99		Ċ	
	MOTA	10201	CEL	. ENE	111	U		2001	00.001	23			_	

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ATOM
           18289
                  ·CZ
                      PHE E
                               8
                                      19.763 63.746
                                                        9.316 1.00 83.35
     MOTA
            18291
                  CE2 PHE E
                               8
                                      18.811
                                               64.520
                                                        9.944
                                                               1.00 82.55
     ATOM
                  CD2 PHE E
           18293
                               8
                                      17.841
                                               63.934
                                                       10.739
                                                               1.00 82.70
     MOTA
           18295
                  С
                       PHE E
                               8
                                      15.507
                                               60.437
                                                       10.291
                                                               1.00 85.47
     ATOM
           18296
                       PHE E
                  0
                               8
                                      16.608
                                               59.978
                                                        9.946
                                                               1.00 83.09
                                                                                     0
                              . 8
10
                  OXT PHE E
     MOTA
           18297
                                    14.521
                                               59.767
                                                        9.937
                                                               1.00 89.34
                                                                                     0
     ATOM
           18298
                       GLU F
                                              14.124 47.515
                  N
                               1
                                      40.126
                                                               1.00 62.65
                                                                                     N
     ATOM
           18300
                      GLU F
                  CA
                                              14.895
                               1
                                      39.361
                                                       48.535
                                                               1.00 57.33
                                                                                     C
     ATOM
           18302
                  CB
                      GLU F
                                      37.879
                                              14.527
                               1
                                                       48.449
                                                               1.00 55.81
     ATOM
           18305
                  CG
                      GLU F
                               1
                                      36.898
                                              15.591
                                                       48.922
                                                               1.00 53.48
15
     MOTA
           18308
                  CD
                      GLU F
                               1
                                      35.432
                                              15.241
                                                       48.626
                                                               1.00 57.95
                                    35.172
     ATOM
           18309
                  OE1 GLU F
                               1
                                              14.718
                                                       47.492
                                                               1.00 57.16
                                                                                     0
     ATOM
           18310
                  OE2 GLU F 1
                                      34.540
                                              15.499
                                                       49.515
                                                               1.00 46.53
                                                                                     0
     ATOM
                       GLU F
           18311
                  С
                               1
                                      39.838 14.584
                                                       49,925
                                                               1.00 56.46
                                                                                     C
     ATOM
                       GLU F
           18312
                  .0
                               1
                                      39.954 13.421
                                                       50.262
                                                               1.00 59.04
                                                                                     0
20
     ATOM
           18315
                       VAL F
                  N
                               2
                                      40.171 . 15.626
                                                       50.694 1.00 52.85
                                                                                     N
     ATOM
           18317
                  CA
                      VAL F
                               2
                                      40.258 15.529
                                                       52.154
                                                              1.00 48.66
                                                                                     C
                      VAL F
                             . 2
    . .ATOM
           18319
                  ·CB
                                      41.331 16.368
                                                       52.682
                                                               1.00 45.45
                                                                                     C
     MOTA
           18321
                  CG1 VAL F
                               2
                                      42.586 15.583
                                                       52.593
                                                              1.00 48.71
                                                                                     C
     ATOM
           18325
                  CG2 VAL F
                                                       51.885
                               2
                                      41.395 17.658
                                                              1.00 48.21
                                                                                     C
25
     MOTA
           18329
                  С
                      VAL F
                               2
                                      39.011 15.976
                                                       52.885
                                                              1.00 45.82
                                                                                     C
     MOTA
           18330
                  0 .
                      VAL F
                               2
                                      38.300
                                              16.826
                                                       52.430
                                                              1.00 52.38
                                                                                     0
     MOTA
           18331
                      ASN F
                  N
                               3
                                      38.762
                                              15.399
                                                       54.047
                                                               1.00 47.13
                                                                                   · N
     ATOM
           18333
                      ASN F
                  CA
                               3
                                      37.566
                                              15.702
                                                       54.814
                                                               1.00 48.46
                                                                                     C
     ATOM
           18335
                      ASN F
                                      36.425
                  CB
                               3
                                              14.705
                                                       54.512
                                                               1.00 46.45
                                                                                     С
30
     ATOM
           18338
                      ASN F
                  CG
                               3
                                      35.499
                                              15.178
                                                       53.371
                                                               1.00 48.95
     ATOM
           18339
                  OD1 ASN F
                               3
                                      34.662 16.042
                                                       53.600
                                                               1.00 56.94
    ATOM
           18340
                  ND2 ASN F
                                     35.637
                                              14.599
                                                       52.147
                                                               1.00 41.31
                                                                                    N
     ATOM
           18343
                  С
                      ASN F
                               3
                                      37.938 15.676
                                                       56.289
                                                               1.00 48.81
                                                                                    С
     ATOM
           18344
                  0
                      ASN F
                               3
                                      37.884 14.650
                                                      56.945
                                                              1.00 46.42
                                                                                    0
35
    · ATOM
           18345
                  0
                      LOL F
                               4.
                                    39.109 18.145
                                                      59.529
                                                               1.00 30.33
                                                                                    0
     ATOM
           18346
                  С
                      LOL F
                               4
                                      39.139 16.727
                                                      59.642
                                                               1.00 37.57
                                                                                    С
     MOTA
           18347
                  CA
                      LOL F
                               4
                                      39.449
                                              15.978
                                                      58.340
                                                               1.00 34.22
     ATOM
           18348
                  N
                      LOL F
                               4
                                      38.607
                                              16.653
                                                      57.414
                                                              1.00 33.81
     MOTA
           18349
                  CB
                      LOL F
                               4
                                      40.854
                                              16.178
                                                      57.816
                                                              1.00 29.74
                                                                                    С
40
     ATOM
           18350
                  CG
                      LOL F
                               4
                                      41.230
                                              14.854
                                                      57.136
                                                               1.00 42.88
                                                                                    C
     ATOM
           18351
                  CD2 LOL F
                                      40.898 13.685
                             . 4
                                                      58.067
                                                               1.00 44.40
                                                                                    C
     ATOM
           18352
                  CD1 LOL F
                                     42.690 14.689
                               4
                                                      56.716
                                                              1.00 33.62
                                                                                    С
     ATOM
           18353
                  0
                      ALQ F
                               5
                                      37.076 16.340
                                                      61.729
                                                              1.00 51.12
                                                                                    0
     MOTA
           18354
                  C
                      ALQ F
                               5
                                      37.482 17.448
                                                      61.387
                                                              1.00 44.19
                                                                                    C
45
     ATOM
           18355
                  CA
                      ALQ F
                               5
                                      37.023 17.885
                                                      60.039
                                                              1.00 45.38
                                                                                    С
     ATOM
           18356
                      ALQ F
                  CM
                               5
                                      37.387 16.833
                                                      58.971
                                                              1.00 30.19
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	MOTA	18387	CA	PHE	F	8	33.718	14.541	67.716	1.00	67.25		С
	ATOM	18389	CB	PHE	F	8	34.303	15.837	68.301	1.00	68.83		·C
	ATOM	18392	CG	PHE	F	8	33.612	16.393	69.544	1.00	64.14		C,
	ATOM.	18393	CD1	PHE	F	8	32.493	17.192	69.441	1.00	65.62		C
10	ATOM	18395	CE1	PHE	F	8	31.873	17.724	70.583	1.00	64.20		С
	MOTA	18397	CZ	PHE	F	8	32.376	17.472	71.840	1.00	63.31		С
	MOTA	18399	CE2	PHE	F	8	33.496	16.688	71.971		65.43		C
	MOTA	18401	CD2	PHE	F	8	34.123	16.150	70.817		66.04		С
	ATOM	18403	С	PHE	F	8	32.209	14.659	67.761		71.68		С
15	ATOM	18404	0	PHE	F	8	31.610	14.612	68.854		73.64	•	0
	ATOM	18405	OXT	PHE	F	8	31.569	14.808	66.717		76.55		0
	MOTA	18406	0	HOH	W	1	39.700	13.653	43.690	1.00	64.49		0
	ATOM	18409	0 .	HOH	W	2	17.999	-0.835	18.526		57.08		0
,	MOTA	18412	0	HOH	W	3	-2.213	39.679	44.264		47.81.		0
20	ATOM	18415	0	HOH	M	4	44.390	21.700	54.614		36.23		0
	MOTA	18418	0	HOH	W	5	44.036	10.520	13.671		20.25		0
	ATOM	18421	0	HOH	W	6	21.081		18.984		79.68		0
	ATOM	18424	0	HOH	W	7	12.954	48.886			47.92		0
	ATOM	18427	0	НОН		8	8.570	89.322	9.495		42.50		0
25	ATOM	18430	0	HOH	W	9	25.965		-10.244		58.04		0
	MOTA	18433	σ	НОН		10	11.743	63.828	30.252		60.50		0
	ATOM	18436	0	НОН		11	-0.897		42.929	•	57.91		0
	ATOM	18439	0	НОН		12	52.750	29.899	42.854		71.96		0
	MOTA	.18442	0	нон		13	31.267	56.125	22.788		67.37		0
30	MOTA	18445	0	HOH		14	-0.501	17.272	5.350				0
	MOTA	18448	0	НОН		15	19.139	31.098	19.928		53.73		0
	ATOM	18451	0	нон		16	29.653	40.187	36.475		51.39		0 .
	MOTA	18454	0	НОН		17	1.702	54.764			59.48		0
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35	MOTA	18460	0	НОН		19	10.345	16.962	33.276		66.13		0
	ATOM	18463	0	нон		20	9.735	17.583	-5.490		62.55		0
	ATOM	18466	0	НОН		21	16.189	57.395	15.723		60.50		0
	ATOM	18469	0	нон		22		79.168	18.933		43.39		Ö
40	MOTA	18472	0	НОН		23	26.061	-0.244	12.926		35.89 60.98		Ö
40	MOTA	18475	0	НОН		24	21.349		-14.919				Ö
	MOTA	18478	0	HOH		25	-4.354		53.329		77.11 46.27		Ö
	ATOM	18481	0	HOH		26	46.391 5.794	31.873	42.449 30.466				Ö
٠	ATOM	18484	0	HOH		27		14.925	53.506		56.03 60.88		ő
45	ATOM	18487	0	нон нон		28 29	18.066 34.788	33.687 61.731	39.462		47.79		Ö
.43	ATOM	18490	0			30	21.025	22.947	1.341		59.51		O.
	ATOM	18493	0	HOH		31		23.886	38.354		45.81		Ö
•	MOTA	18496 18499	0	НОН		32	39.142	5.166	3.509		66.57		ŏ
			-	НОН		33	60.666	20.142	53.793		44.92		o
50 .	ATOM ATOM	18502 18505	.0	НОН		34	. 42.265	8.229	-0.588		60.46	•	ŏ
JU	ATOM		_	НОН		35	32.860	14.034	60.875		60.98		ŏ
		18508 18511	0	НОН		36	32.941	17.022	57.493		38.19		ŏ.
	ATOM.	18514	0.	нон		37	29.695	61.886	47.641		59.00		ŏ
	ATOM ATOM	18517	Ö	НОН		38		-12.279	-2.746		45.53		ō
55	ATOM	18520	Ö	нон		39		-14.843	19.171		65.48		Ō
55	ATOM	18523	Ö	нон		40	24.064		-21.588		70.17		Ö
	ATOM	18526	0	нон		41	23.715	82.758	18.726		35.41		ŏ
	ATOM	18529	0	НОН		42		-13.020	29.129		52.35		ō
	ATOM	18532	0	НОН	•	43		-15.675	-0.741		53.72	•	ō
60	ATOM	18535	o	нон		44	27.524	78.411	40.703		48.20		ō
	ATOM	18538		НОН		45	31.107	72.075	37.162		47.99		ō
	011	10000	. ~		••								-

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           18862
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     ATOM
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     MOTA
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5	ATOM	18883	Ο.	HOH W 160	45.628	3.345	77.459	1.00 52.32	0
	ATOM	18886	0	HOH W 161	49.305	24.574	45.364	1.00 73.80	0
	ATOM	18889	0	HOH W 162	23.302	22.739	1.013	1.00 64.58	0
•	MOTA	18892	0	HOH W 163	4.901	31.457	31.801	1.00 63.61	0
	ATOM	18895	0	HOH W 164	35.668	9.733	38.971	1.00 57.20	0
10	ATOM	18898	0	HOH W 165	50.588	20.385	73.103	1.00 65.81	0
	ATOM	18901	0	- HOH W 166	27.437	13.505	15.130	1.00 54.05	0
	ATOM	18904	0	HOH W 167	18.140	44.428	69.479	1.00 60.04	0
	ATOM	18907	0	HOH W 168	20.428	61.835	21.571	1.00 50.20	0
	ATOM	18910	0	HOH W 169	16.346	20.786	61.900	1.00 68,58	. 0
15	ATOM	18913	0	HOH W 170	10.022	-16.733	-3.299	1.00 45.71	. 0
	ATOM	18916	o	HOH W 171	52.508	6.294	75.257	1.00 53.77	0
	ATOM	18919	0	HOH W 172	58.749	6.101	66.320	1.00 46.84	0
	ATOM	18922	0	HOH W 173	28.460	-0.709	0.570	1.00 49.98	0
•	ATOM	18925	0	. HOH W 174	10.291	60.292	8.525	1.00 55.76	0
20	ATOM	18928	0	HOH W 175	4.095	2.945	15.154		0
	ATOM	18931	0	HOH W 176	7.244	-13.384	-5.254	1.00 48.74	. 0
	MOTA	18934	0	.HOH W 177	32.377	-16.618	-4.059	1.00 44.28	0
	MOTA	18937	0	HOH W 178	47.649	0.734	67.335	1.00 49.13	0
	MOTA	18940	0	HOH W 179	12.789	47.261	47.980	1.00 63.48	0
25	MOTA	18943	0	HOH W 180	5.446	-15.480	-4.436	1.00 57.50	0
	ATOM	18946	0	HOH W 181	9.087	37.020	24.095	1.00 67.94	0
	. ATOM	18949	0	HOH W 182	20.864	-8.162	29.795	1.00 49.49	0
	ATOM	18952	O	HOH W 183	43.991	-1.427	62.252	1.00 55.02	0

* * *

Having thus described in detail preferred embodiments of the present invention, it is to be understood that the invention defined by the appended claims is not to be limited by particular details set forth in the above description as many apparent variations thereof are possible without departing from the spirit or scope thereof.

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WHAT IS CLAIMED IS:

1. A catalytic domain of BACE or a form of BACE that is suitable for crystallization with the correct disulphide bonding that eliminates the need for refolding and/or an apo-BACE crystal or an apo-BACE crystal that can be soaked to give complexes and/or a crystalline form of BACE having crystals that are grown at or near the physiological pH of the enzyme or between about pH 5.6 and about pH 5.8 and/or a BACE crystal having a space group of C2 and/or a BACE crystal having cell dimensions of a= 236.63Å or 236.63Å ± standard deviation (0.2Å) or 236.63Å \pm 3.0Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or $105.02\text{Å} \pm 3.0\text{Å}$, and c= 62.59Å or $62.59\text{Å} \pm \text{standard deviation}$ (0.2Å) or 62.59Å \pm 3.0Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm 3.0Å, b= 107.4Å \pm standard deviation (0.2Å) or $107.4\text{Å} \pm 3.0\text{Å}$, and c= 60.4Å or $60.4\text{Å} \pm \text{standard deviation}$ (0.2Å) or $60.4\text{\AA} \pm 3.0\text{\AA}$ and $\beta=101.89^{\circ}$ or $101.89^{\circ} \pm \text{standard deviation } (0.2^{\circ})$ or between 101° and 108° and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing; and/or having a space group transition from C2 to P21 together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P21 form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand; and/or a BACE crystal having a resolution better than 3 Å; and/or a BACE crystal having the structure defined by the co-ordinates of Table 5.

- 2. A BACE crystal having the structure defined by the co-ordinates of Table 5.
- 3. An apo-BACE crystal grown at or near the physiological pH of the enzyme.
- 4. An apo-BACE crystal or an apo-BACE crystal that can be soaked to give complexes.
- 5. A crystalline form of BACE or a functional portion thereof having crystals that are grown at or near the physiological pH of the enzyme.
- 6. The crystalline form of BACE or functional portion thereof of claim 6 wherein the crystals are grown at a pH between about pH 5.6 and about pH 5.8

7. A crystalline form of BACE or a functional portion thereof having a space group of C2 and cell dimensions of a= 236.63Å or 236.63Å \pm standard deviation (0.2Å) 236.63Å \pm 3.0Å, b= 105.02Å or 105.02Å \pm standard deviation (0.2Å) or 105.02Å \pm 3.0Å, and c= 62.59Å or 62.59Å \pm standard deviation (0.2Å) or 62.59Å \pm 3.0Å and β =101.32° or 101.32° \pm standard deviation (0.2°) or between 101° and 108° with the asymmetric unit of the crystal containing three copies of BACE or cell dimensions a= 238.3Å or 238.3Å \pm standard deviation (0.2Å) or 238.3Å \pm 3.0Å, b= 107.4Å or 107.4Å \pm standard deviation (0.2Å) or 107.4Å \pm 3.0Å, and c= 60.4Å or 60.4Å \pm standard deviation (0.2Å) or 60.4Å \pm 3.0Å and β =101.89° or 101.89° \pm standard deviation (0.2°) or between 101° and 108° and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having an X-ray diffraction pattern corresponding to or resulting from any or all of the foregoing and/or having a space group transition from C2 to P2₁ together with an increase in the number of copies of the molecule in the asymmetric unit, while the cell dimensions and the packing of the P2₁ form are closely related to those of the C2 crystal form, on soaking the apo-BACE crystal with a ligand.

- 8. A crystalline form of BACE or a functional portion thereof that has an active site containing one or more ligands other than the natural substrate or the substrate that occurs naturally or physiologically within the active site.
- 9. A method for ligand screening or identification comprising exposing the BACE crystals of any one of claims 2-8 to one or more test samples, and determining whether a ligand-BACE complex is formed.
- 10. The method of claim 9 wherein the BACE protein or functional portion thereof is exposed to the test samples by co-crystallizing the BACE protein or functional portion thereof in the presence of the one or more test samples.
- 11. The method of claim 9 wherein the BACE of claims 2-8 is soaked in a solution of one or more test samples
- 12. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the

atoms in the BACE catalytic domain, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

13. A compound having a chemical structure selected using the methods of claims 9-12, said compound being a modulator of BACE

- 14. A BACE protein or functional portion thereof comprising amino acid sequences of the catalytic domain that crystallize to the crystalline structure of claim 7, or to a structure that mimics that crystalline structure.
- 15. A BACE protein or functional portion thereof which, when compared to wild-type BACE or BACE of Genbank accession P56817 has one or more mutations or truncations to prevent glycosylation or facilitate crystallization and/or the growth of ordered, well-diffracting crystals.
- 16. The BACE protein or functional portion thereof of claim 15, which when compared with Genbank accession P56817 has one or more of: a mutation at amino acid ("aa") 153, a mutation at aa 172, a mutation at aa 223, a mutation at aa 354, and one or more truncations.
- 17. The BACE protein or functional portion thereof of claim 16 wherein each of the mutations is asparagine to glutamine.
- 18. The BACE protein or functional portion thereof of claim 16 wherein the truncation results in a BACE extending from Thr 22 to Ser 453, with reference to Genbank Accession P56817.
- 19. The BACE protein or functional portion thereof of claim 16 wherein all of the mutations are present and each is asparagine to glutamine and there is a truncation resulting in a BACE extending from Thr 22 to Ser 453, with reference to Genbank Accession P56817.
- 20. The BACE protein or functional portion thereof of any one of claims 14-19 further including any one or more of: a tag to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium; and a tag to allow differentiation of species arising from incomplete pro-peptide cleavage.
- 21. The BACE protein or functional portion thereof of claim 20 wherein the tag to facilitate purification is a HIS tag, the non-BACE signal sequence is a baculovirus signal sequence, and the tag to allow differentiation of species is a FLAG tag.
- 22. The BACE protein or functional portion thereof of claim 21 wherein all of the tag to facilitate purification, the non-BACE signal sequence and the tag to allow differentiation are present.

23. A BACE protein or functional portion thereof containing any one or more of: a tag to facilitate purification; a non-BACE signal sequence to facilitate or increase secretion of the protein into cell culture medium; and a tag to allow differentiation of species arising from incomplete pro-peptide cleavage.

- 24. The BACE protein or functional portion thereof of claim 23 wherein the tag to facilitate purification is a HIS tag, the non-BACE signal sequence is a baculovirus signal sequence, and the tag to allow differentiation of species is a FLAG tag.
- 25. The BACE protein or functional portion thereof of claim 24 wherein all of the tag to facilitate purification, the non-BACE signal sequence and the tag to allow differentiation are present.
- 26. An isolated nucleic acid molecule encoding a BACE protein or functional portion thereof of any of claims 14-25 or a functional portion thereof.
- 27. The isolated nucleic acid molecule of claim 26 that has a reduced GC content via silent mutations from nucleotide sequences derived from wild-type BACE that would also encode the BACE protein.
 - 28. A vector or cell comprising or expressing the nucleic acid molecule of claim 26.
 - 29. A vector or cell comprising or expressing the nucleic acid molecule of claim 27.
- 30. The vector or cell of claim 28 which is a viral vector or a bacterial vector or a mammalian cell or a DNA plasmid.
- 31. The vector or cell of claim 29 which is a viral vector or a bacterial vector or a mammalian cell or a DNA plasmid.
- 32. The vector or cell of claims 30 or 31 which is a baculovirus vector or an insect cell.
- 33. The vector or cell of claim 26 further including a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
- 34. The vector or cell of claim 27 further including a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
- 35. The vector or cell of claims 33 or 34 wherein the enhancer is a prohormone convertase.

36. The vector or cell of claim 35 wherein the prohormone convertase is furin.

- 37. A vector or cell comprising a nucleic acid molecule encoding a BACE protein or functional portion thereof and a nucleic acid molecule encoding an enhancer that enhances in the particular vector or cell system the total amount of BACE produced and/or increases the fraction of processed protein.
 - 38. The vector or cell of claim 37 wherein the enhancer is a prohormone convertase.
- 39. A kit for producing the vector or cell of claim 37 containing separately packaged nucleic acid molecules comprising (i) a BACE-protein encoding nucleic acid molecule and (ii) a nucleic acid molecule encoding the enhancer.
- 40. A method for obtaining a BACE protein comprising expressing a nucleic acid molecule according to any of claims 26 or 27 or the nucleic acid molecule of the vector or cell of any of claims 28 to 34 or 37.
- 41. A method for obtaining a BACE protein comprising expressing the nucleic acid molecule of the vector or cell of claim comprising expressing in a vector or cell the nucleic acid molecules of the kit of claim 39.
- 42. A method for crystallizing a BACE protein or functional portion thereof comprising dissolving a BACE protein according to any one of claims 14-25 in a suitable solvent and crystallizing the same either in the presence or absence of an inhibitor; wherein said method optionally further includes producing the BACE recombinantly or by expression thereof by a vector, recovering the BACE so produced, and growing crystals from the recovered BACE.
 - 43. The method of claim 42 wherein the inhibitor is OM99-2.
- 44. A method for determining the crystal structure of a BACE protein or functional portion thereof comprising obtaining crystals of a BACE protein according to any one of claims 14-25 and obtaining an x-ray diffraction pattern thereof.
- 45. A method for ligand screening and design or identification comprising exposing the BACE crystals of a BACE protein or functional portion thereof to one or more test samples, and determining whether a ligand-BACE complex is formed; wherein the BACE or functional portion thereof has an unoccupied active site and is as claimed in any one of claims 5-8.

46. The method of claim 45 wherein the BACE is exposed to the test samples by either co-crystallizing the BACE or functional portion thereof in the presence of the one or more test samples or soaking the BACE or a functional portion thereof in a solution of one or more test samples.

47. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain or functional portion thereof of any one of claims 5-8, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE

to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

- 48. A ligand identified in any of the methods of claims 45-47.
- 49. An assay comprising a BACE protein or functional portion thereof of any one of claims 14-25, and means to determine whether a compound is a modulator of BACE.
- 50. An antibody elicited by a BACE protein or functional portion thereof of any one of claims 14-25.
- 51. An inhibitor of a BACE protein or functional portion thereof of any one of claims 14-25.
 - 52. A composition comprising the inhibitor of claim 51.
 - 53. A composition comprising the ligand of claim 48.
 - 54. A composition comprising the ligand of claim 13.
 - 55. A composition comprising a product from the assay of claim 49.
- 56. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51.
- 57. A method for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 13.
- 58. A method for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 48.
- 59. A BACE which comprises an amino acid sequence of SEQ ID NO: 5 or an amino acid sequence having greater than 98.8% identity with SEQ ID NO:5.
 - 60. The BACE of claim 59 having the amino acid sequence of SEQ ID NO:5.
 - 61. A nucleic acid molecule encoding the BACE of claim 59 or 60.
- 62. An isolated nucleic acid molecule comprising a sequence of SEQ ID NO: 4 or 10 or a sequence having greater than 95.6% identity with SEQ ID NO: 4 or 10.
- 63. The isolated nucleic acid molecule of claim 62 having the sequence of SEQ ID NO:4.

64. The isolated nucleic acid molecule of claim 63 having the sequence of SEQ ID NO:10.

- 65. A vector or cell comprising the isolated nucleic acid molecule of any one of claims 62-64.
 - 66. The vector or cell of claim 65 which is a baculovirus vector or an insect cell.
 - 67. An inhibitor of the BACE of any one of claims 59 or 60.
 - 68. An antibody elicited by the BACE of any one of claims 59 or 60.
- 69. A method for ligand screening and design or identification comprising exposing the BACE crystals of a BACE protein or functional portion thereof to one or more test samples, and determining whether a ligand-BACE complex is formed; wherein the BACE or functional portion thereof has an unoccupied active site and is as claimed in any one of claims 59 or 60.
- 70. The method of claim 69 wherein the BACE is exposed to the test samples by either co-crystallizing the BACE or functional portion thereof in the presence of the one or more test samples or soaking the BACE or a functional portion thereof in a solution of one or more test samples.
- 71. A computer-assisted method for identifying or designing potential ligands to fit within the catalytic domain of BACE or a functional portion thereof:

comprising using a programmed computer comprising a processor, a data storage system, an input device, and an output device, the steps of: (a) inputting into the programmed computer through said input device data comprising the three-dimensional co-ordinates of a subset of the atoms in the BACE catalytic domain or functional portion thereof of any one of claims 59 or 60, optionally with structural information from ligand-BACE complexes, thereby generating a data set; (b) comparing, using said processor, said data set to a computer database of chemical structures stored in said computer data storage system; (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said data set; (d) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said data set and (e) outputting to said output device the selected chemical structures having a portion similar to said data set; and optionally synthesizing one or more of the selected chemical structures; and further optionally contacting said synthesized

selected chemical structure with BACE to ascertain whether said synthesized chemical structure is a ligand that fits within the catalytic domain of BACE and/or inhibits BACE; or,

comprising: providing the structure of BACE as defined by the co-ordinates of Table 5, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the structure of the BACE of Table 5; or,

comprising: providing the co-ordinates of at least two atoms of Table 5 of BACE ("selected co-ordinates"), providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the selected co-ordinates of BACE; or,

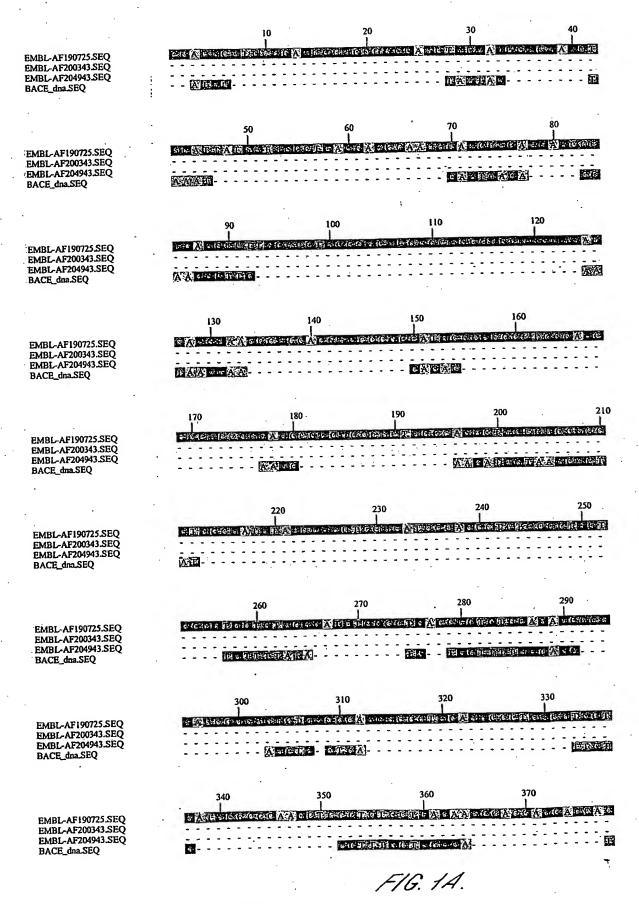
comprising: providing the co-ordinates of at least a sub-domain of BACE, providing the structure of a candidate modulator molecule, and fitting the structure of the candidate to the sub-domain of BACE;

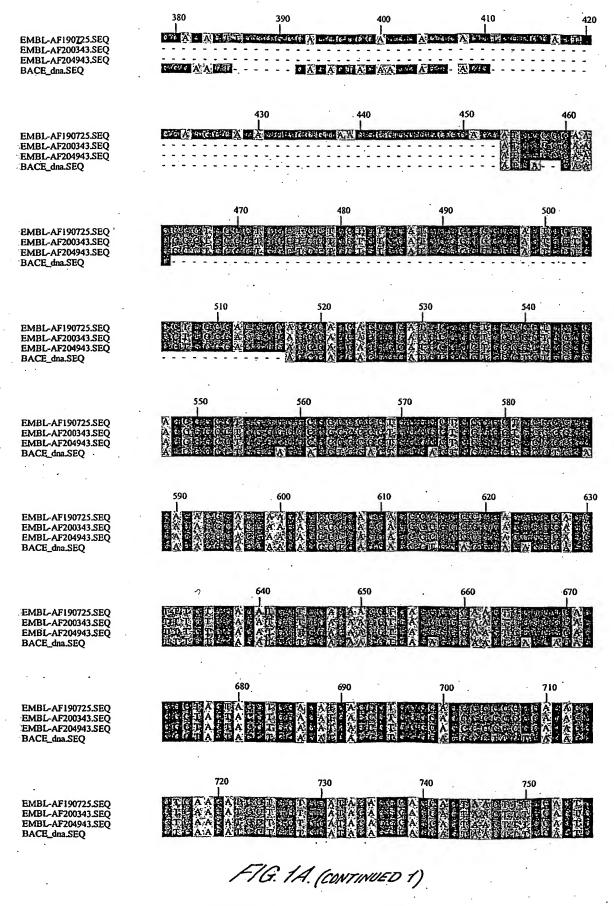
said method optionally further comprising: obtaining or synthesizing the chemical structure or candidate modulator and contacting the chemical structure or candidate modulator with BACE to determine the ability of the chemical structure or candidate to interact with BACE; or obtaining or synthesizing the chemical structure or candidate modulator and forming a complex of BACE and said chemical structure or candidate modulator, and analyzing the complex to determine the ability of said chemical structure or candidate modulator to interact with BACE.

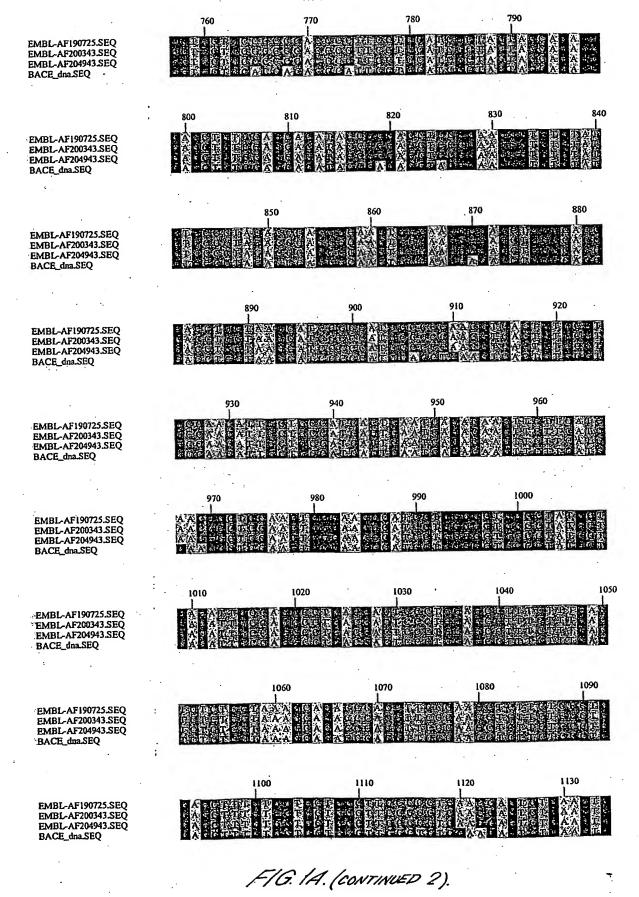
- 72. A ligand identified in any of the methods of claims 68-71.
- 73. An assay comprising a BACE protein or functional portion thereof of any one of claims 58 or 59, and means to determine whether a compound is a modulator of BACE.
 - 74. A composition comprising the inhibitor of claim 67.
 - 75. A composition comprising the ligand of claim 72.
 - 76. A composition comprising a product from the assay of claim 73.
- 77. A method for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof comprising administering an inhibitor of a BACE protein or functional portion thereof as claimed in claim 67.
- 78. A method for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof comprising administering a ligand of claim 72.
- 79. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51 for preparing a composition or medicament for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof.

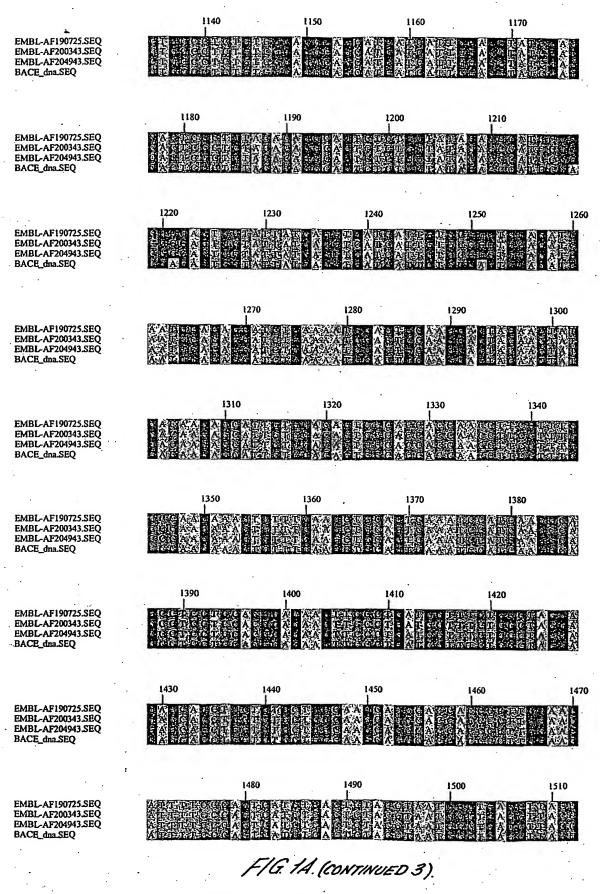
80. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 13 for preparing a composition or medicament for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof.

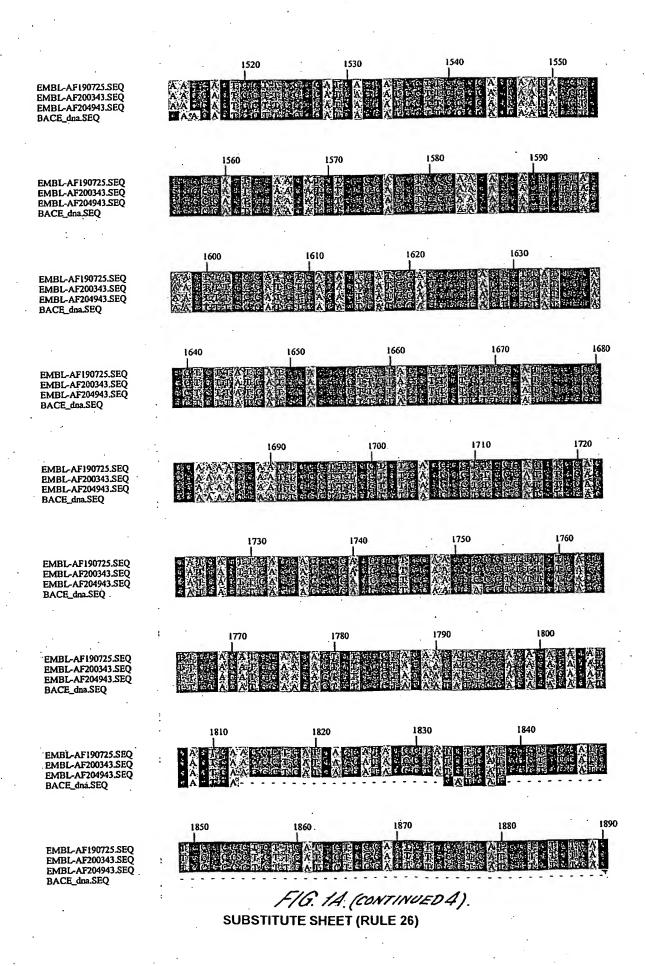
- 81. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 48 for preparing a composition or medicament for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof.
- 82. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 51 for use in therapy.
- 83. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 67 for preparing a composition or medicament for inhibiting BACE or the production of Aβ or fragments thereof or treating AD in an individual in need thereof.
- 84. Use of an inhibitor of a BACE protein or functional portion thereof as claimed in claim 72 for preparing a composition or medicament for inhibiting BACE or the production of $A\beta$ or fragments thereof or treating AD in an individual in need thereof.
- 85. A computer system for generating structures or performing rational compound or drug design for BACE or complexes of BACE with a potential modulator, the system containing either: atomic co-ordinate data according to Table 5, said data defining the three-dimensional structure of BACE or at least one sub-domain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.
- 86. A computer readable media with either: atomic co-ordinate data according to Table 5, said data defining the three-dimensional structure of BACE or at least one sub-domain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.
- 87. A method of doing business comprising providing to a user the computer system of claim 85 or the computer readable media of claim 83 or the three-dimensional structure of BACE or at least one sub-domain thereof, or structure factor data for BACE, said structure factor data being derivable from the atomic co-ordinate data of Table 5.

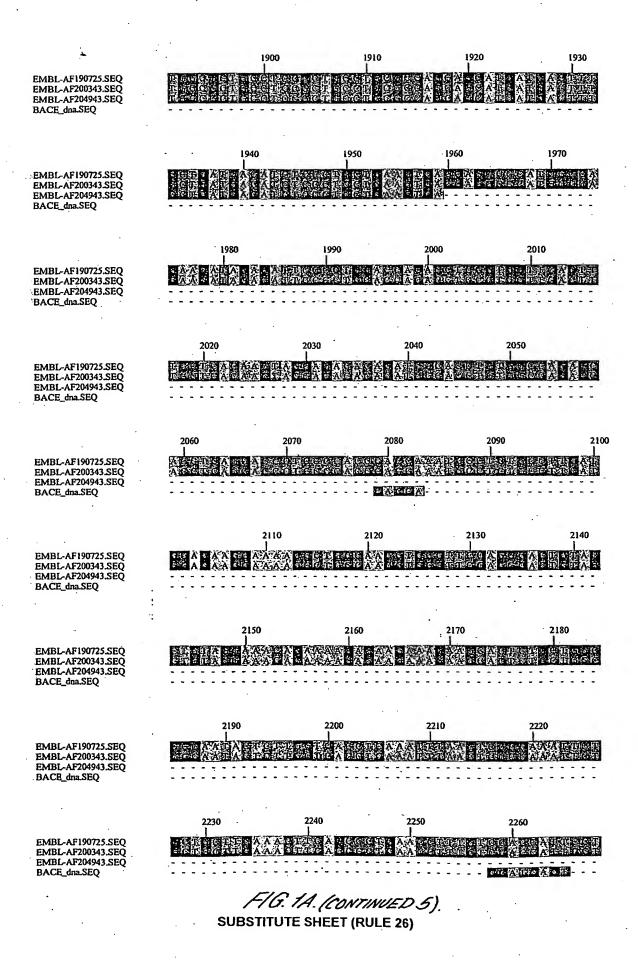












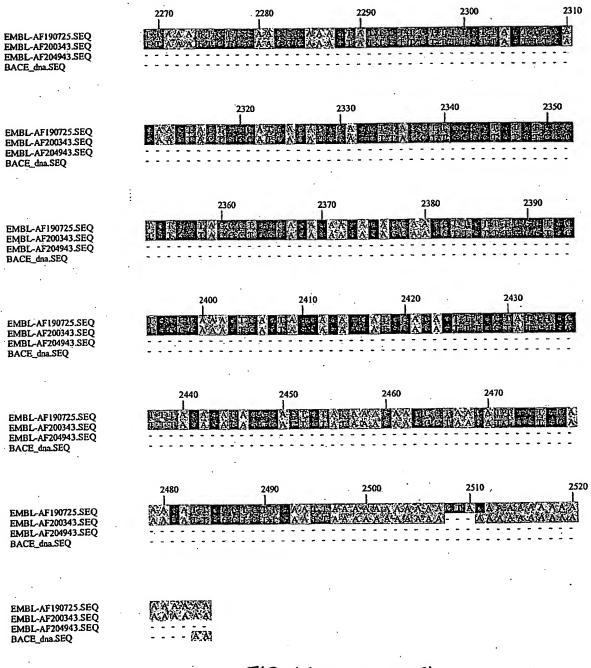


FIG. 1A. (CONTINUED 6).

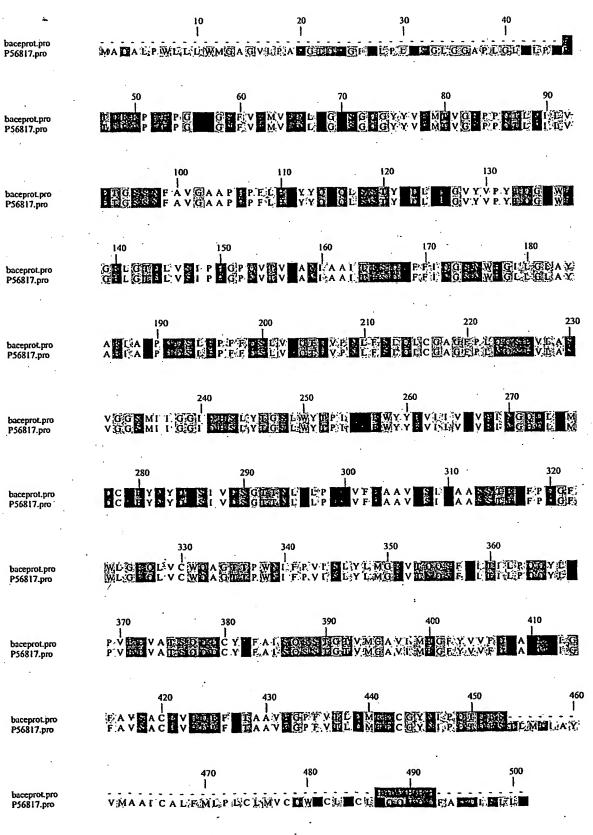


FIG. 18.

ETDEEPEEPG	RRGSFVEMVD	NLRGKSGQGY	YVEMTVGSPP	QTLNILVDTG	SSNFAVGAAP	60
HPFLHRYYOR	QLSSTYRDLR	KGVYVPYTQG	KWEGELGTDL	VSIPHGPQVT	VRANIAAITE	120
SDKFFIQGSN	WEGILGLAYA	EIARPDDSLE	PFFDSLVKQT	HVPNLPSLQL	CGAGFPLQQS	180
EVLASVGGSM	IIGGIDHSLY	TGSLWYTPIR	REWYYEVIIV	RVEINGQDLK	MDCKEANADK	240
SIVDSGTTNL	RLPKKVFEAA	VKSIKAASST	EKFPDGFWLG	EQLVCWQAGT	TPWNIFPVIS	300
LYLMGEVTQQ	SFRITILPQQ	YLRPVEDVAT	SQDDCYKFAI	SQSSTGTVMG	AVIMEGFYVV	360
PDRARKRIGE	AVSACHVHDE	FRTAAVEGPF	VTLDMEDCGY	NIPOTDESHH	HHHH	414

FIG. 2A

GCTTTTGGCAGCAGCTGCTCATTCTGCCTTTGCTGCGGATCCGAATTCAGACTACAAGGACGACGATGACAAGACCCAGC ACGGATCCGCTGCCTCCGCAGCGGCCTGGGAGGAGCTCCACTGGGACTGCGCTGCCTCGAGAGACCGACGAAGAC CCTGAGGAGCCTGGACGGAGAGGCAGCTTTGTGGAGATGGTGGACAACCTGAGAGGCAAGTCAGGACAGGGCTACTACGT GGAGATGACCGTGGGCAGCCCTCCTCAGACGCTCAACATCCTGGTGGATACAGGCAGCAGTAACTTTGCAGTGGTGCTG CACCACACCCATTCCTGCATCGCTACCAGAGGCAGCTGTCCAGCACATACCGAGACCTACGGAAGGGTGTGTATGTG CCCTACACCCAGGCAAGTGGGAAGGAGAGCTGGCACCGACCTGGTAAGCATCCCCCATGGACCTCAAGTCACTGTGCG TGCCAACATTGCTGCCATCACTGAATCAGACAAGTTCTTCATCCAAGGCTCCAACTGGGAAGGCATCCTGGGGCTGGCCT TGGAGGTATCGACCACTCGCTGTACACAGGCAGTCTCTGGTATACACCCATCCGAGGAGGTGGTATTATGAGGTGATCA TTGTGCGAGTGGAGATCAATGGACAGGATCTGAAAATGGACTGCAAGGAGTACAACTATGACAAGAGCATTGTGGACAGT GGCACCACCAACCTTCGTTTGCCCAAGAAAGTGTTTGAAGCTGCAGTCAAATCCATCAAGGCAGCCTCCTCCACGGAGAA GTTCCCTGATGGTTTCTGGCTAGGAGAGCAGCTGGTGTGCTGGCAAGCAGCACCCCCTTGGAACATTTTCCCAGTCA TCTCACTCTACCTAATGGGTGAGGTTACCCAACAGTCCTTCCGCATCACCATCCTTCCGCAGCAATACCTGCGGCCAGTG GAAGATGTGGCCACGTCCCAAGACGACTGTTACAAGTTTGCCATCTCACAGTCATCCACGGGCACTGTTATGGGAGCTGT TATCATGGAGGGCTTCTACGTTGTCTTTGATCGGGCCCGAAAACGAATTGGCTTTGCTGTCAGCGCTTGCCATGTGCACG ATGAGTTCAGGACGCCAGCGGTGGAAGGACCTTTTGTCACCTTGGACATGGAAGACTGTGGCTACAATATTCCACAGACA GATGAGTCACATCATCACCACCATCACTAA

FIG. 2B.

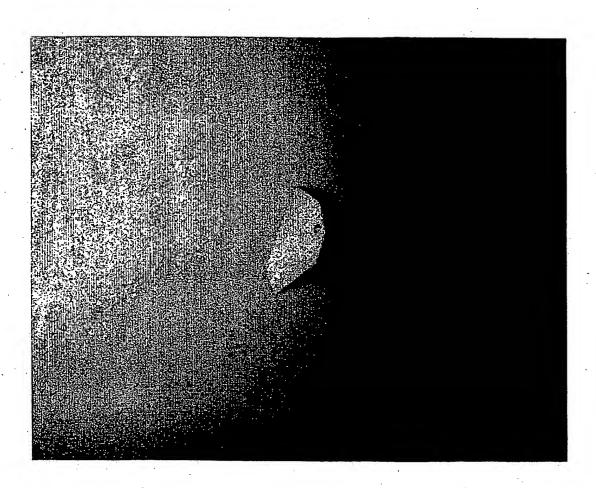


FIG. 3A.

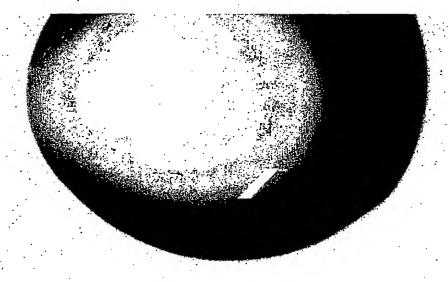


FIG. 3B.

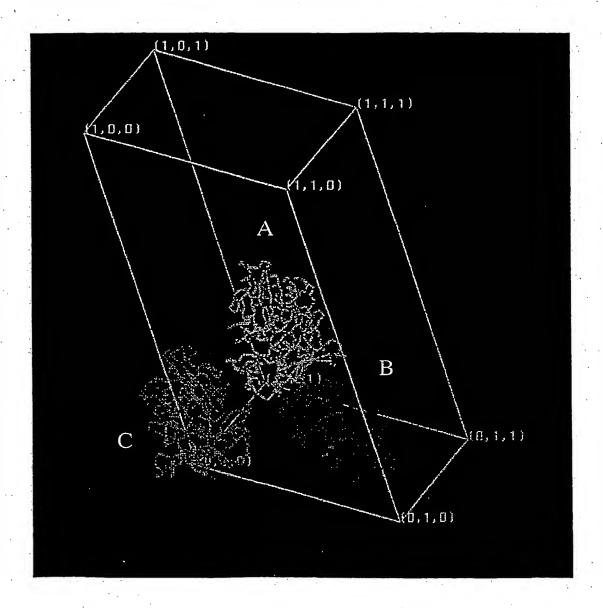


FIG. 4A.

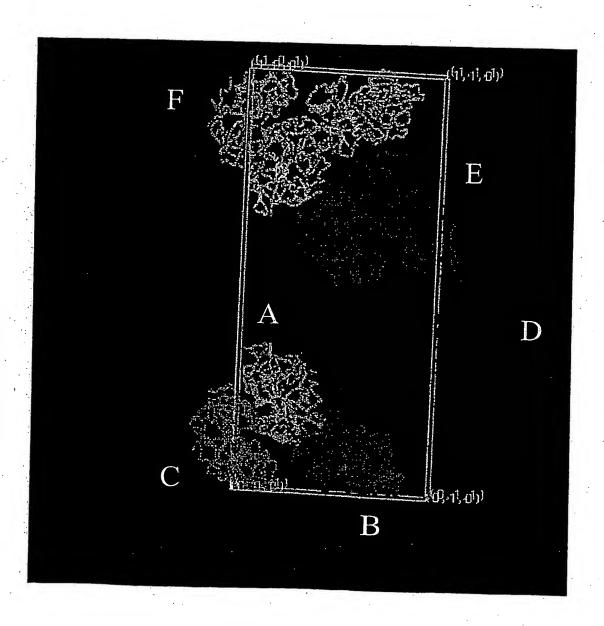
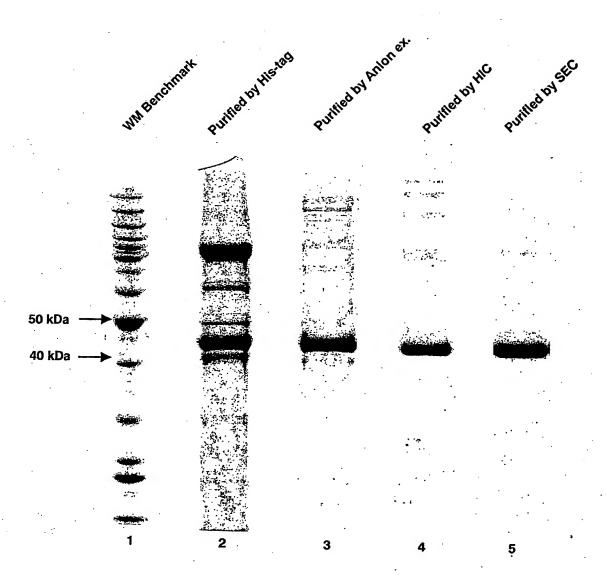
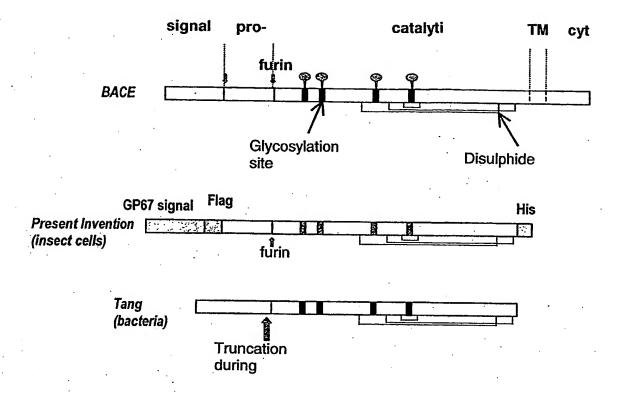


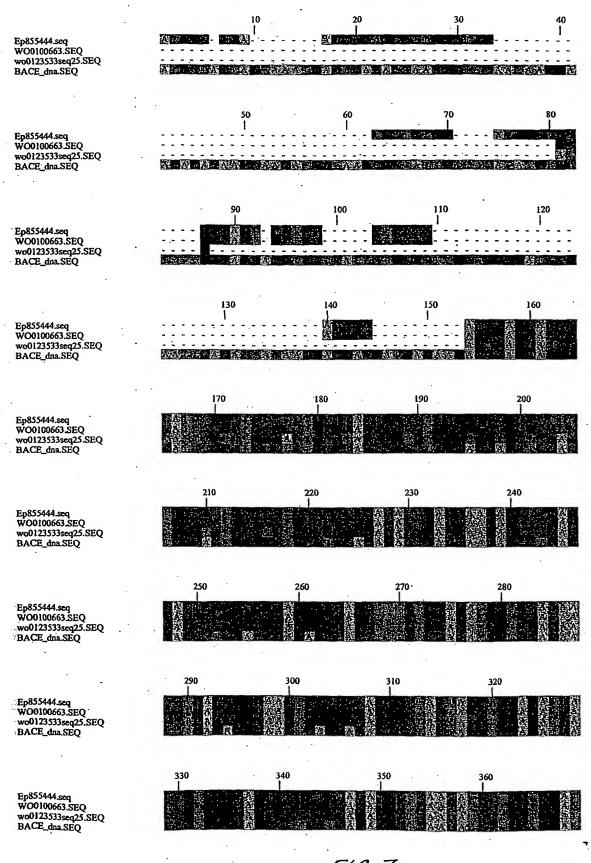
FIG. 4B.



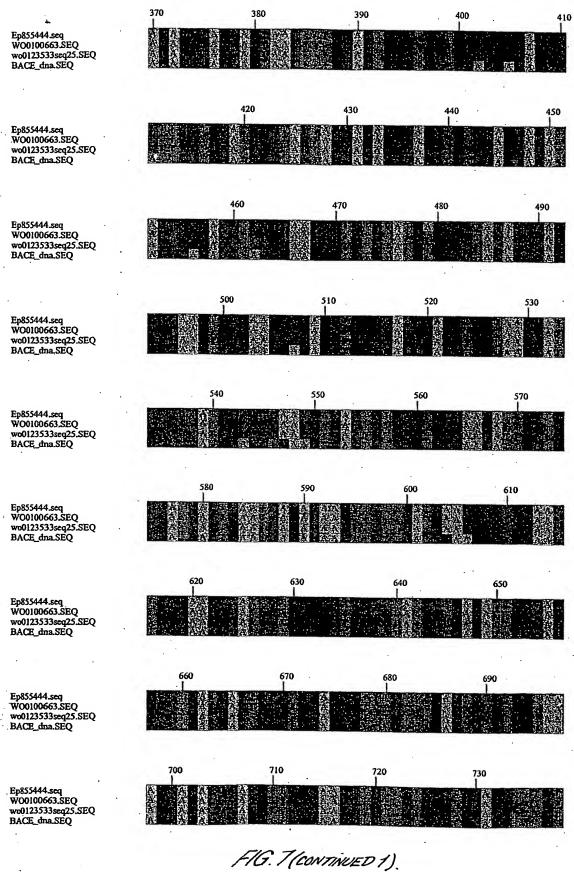
F/G. 5.



F1G. 6.



F/G. 7.
SUBSTITUTE SHEET (RULE 26)



740 750 760 770 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 780 790 800 810 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 830 840 850 860 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 870 880 890 900 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna_SEQ 910 920 930 940 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 950 970 960 980 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 990 1000 1010 1020 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna_SEQ 1030 1040 1050 1060 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ 1070 1080 1090 1100 Ep855444.seq WO0100663.SEQ wo0123533seq25.SEQ BACE_dna.SEQ

FIG. 7 (CONTINUED 2).
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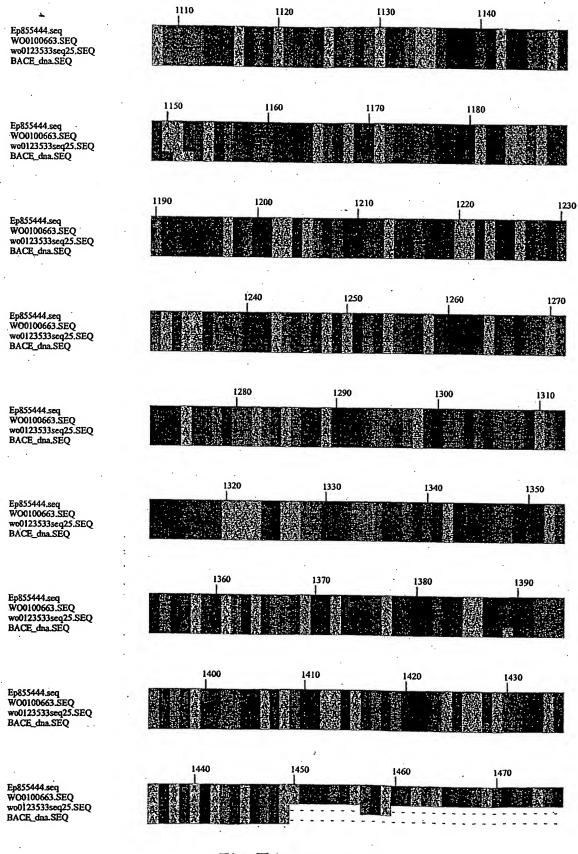
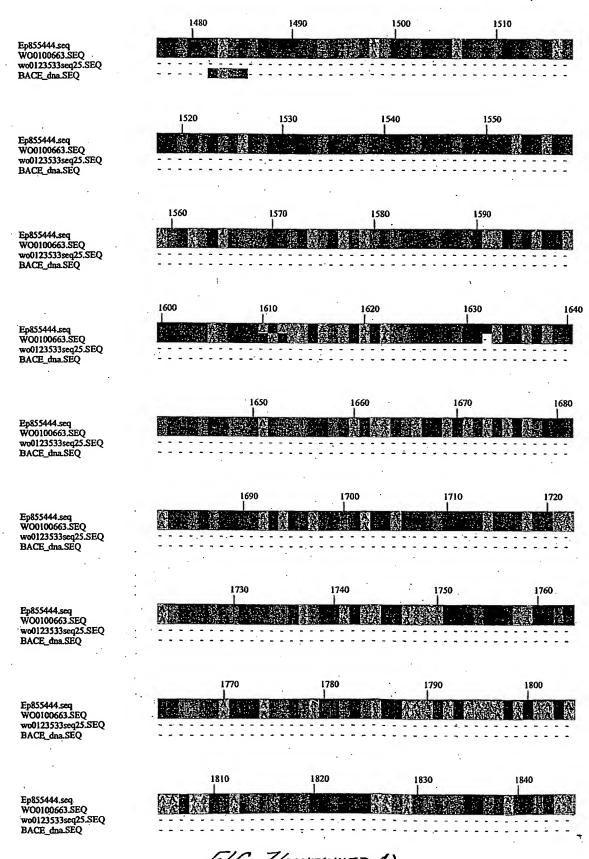
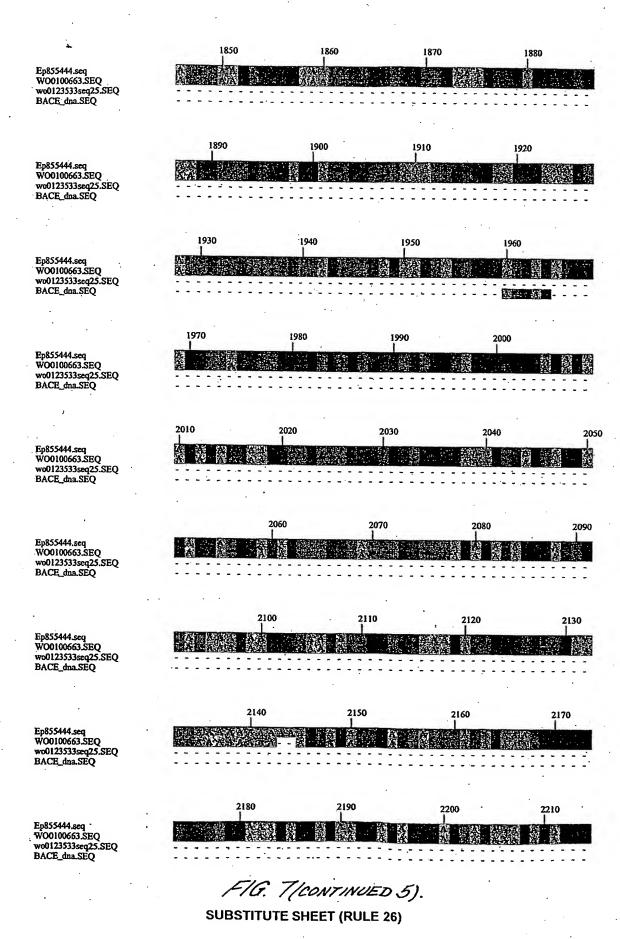
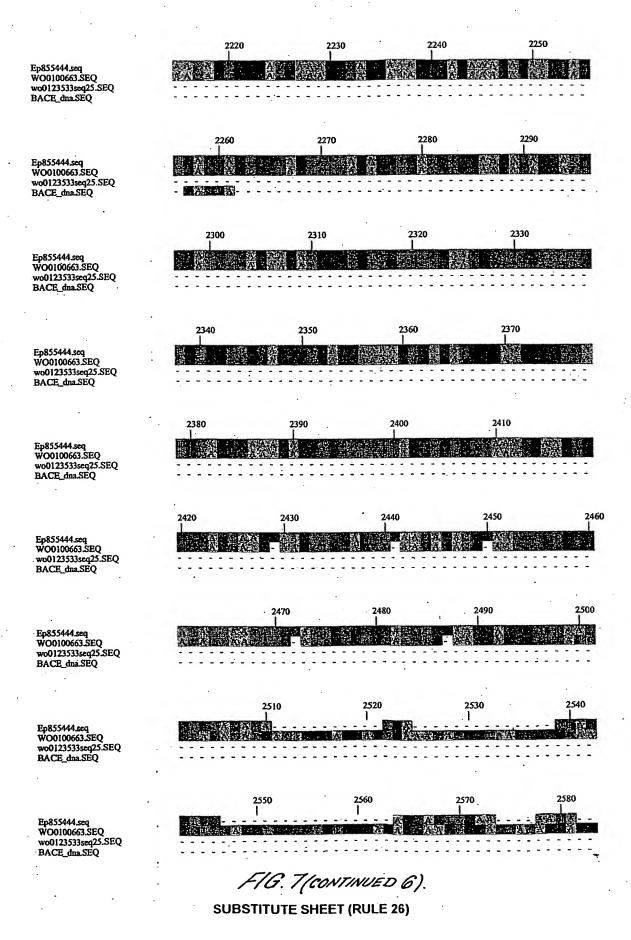


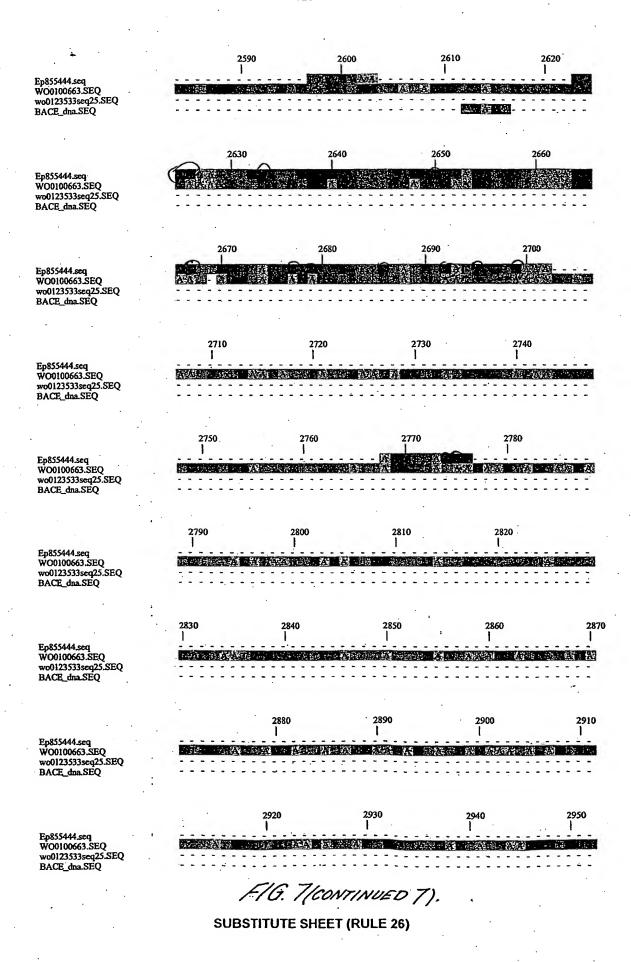
FIG. T(CONTINUED 3).
SUBSTITUTE SHEET (RULE 26)

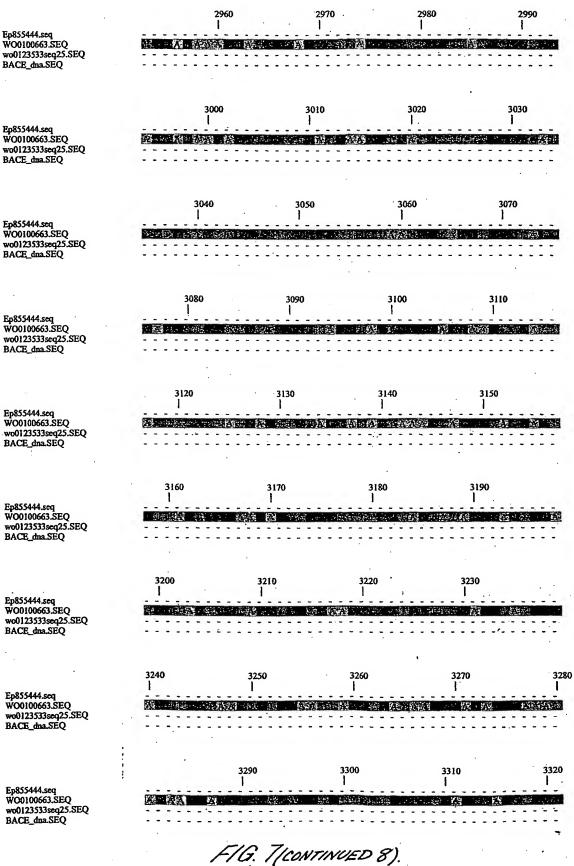


F/G. T/CONTINUED 4).
SUBSTITUTE SHEET (RULE 26)







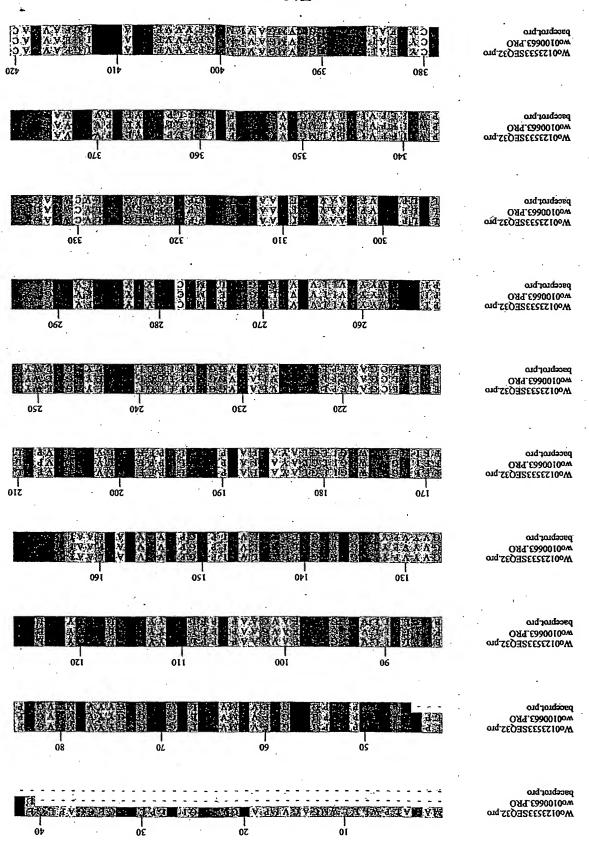


110.1/20001110220)

FIG. T(CONTINUED 9).

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Wo0123533SEQ32.pro wo0100663.PRO baceprot.pro



Wo0123533SEQ32.pro wo0100663.PRO baceprot.pro

FIG. 8(CONTINUED).